

Comments on the U.S. Army Corps of Engineers Report, “CFD Study and Structural Analysis of the Sago Mine Accident”

Murali M. Gadde,
David A. Beerbower,
John A. Rusnak,
Peabody Energy, Saint Louis, MO.

1.0 Introduction

The Mine Safety and Health Administration (MSHA) has recently released the U.S. Army Corps of Engineers study on the Sago mine explosion [1]*. MSHA sought public comments on several issues discussed in the Corps’ study. These comments here specifically address the validity of the assumptions made and the conclusions drawn in the Corps’ study.

In general, we think the Corps’ study was well conducted within the limits of the inputs provided to them. The study also demonstrates the usefulness of computational fluid dynamics (CFD) modeling for studying coal mine explosions. In our opinion, the Corps’ exhaustive CFD modeling of the Sago mine represents the first step in the right direction to address the challenges involved in understanding and mitigating coal mine explosions.

Our research, however, shows that at this point of time, the Corps’ report [1] should not be considered in any anticipated rule making. This is not because there were any major problems with the modeling, but because the right inputs were simply not available to them for conducting such a sophisticated modeling for prescriptive purposes and definitely not to guide the policy. In what follows, we will extensively discuss the reasons behind our conclusion.

Despite the lack of proper inputs, we do believe that the computational fluid dynamics modeling can be used effectively to conduct parametric studies that help understand the effect of different variables on the explosion output. Within the next few years, as we try to develop more reliable inputs and “fine-tune” CFD modeling for coal mine applications, it may be possible to use numerical models for predicting the magnitudes of explosion loading as well.

The work done in the Corp’s report [1] could be separated under two different subject headings:

- CFD modeling
- Structural modeling

In the following sections, we will comment on these two subject matters separately.

2.0 CFD Modeling

In the Sago report, the Corps of Engineers used a sophisticated computational fluid dynamics code called, SAGE. This program was developed by the Los Alamos National Laboratory and

* Reference number given at the end

SAIC [1]. It was mentioned in the report that SAGE has been used for solving a gamut of problems in fluid dynamics, one of which is for simulating reactive flows [1].

In a reactive flow problem, the governing partial differential equations are very complicated to be solved analytically for a majority of the practical problems [2]. Therefore, approximate solutions are sought by using numerical techniques like the finite difference method, the finite volume method etc. Since numerical methods are used to solve the governing equations, the solutions will not be perfectly accurate as is the case with “closed-form” solutions. However, with a *proper* modeling approach, it may be possible to obtain solutions to a reactive flow problem with acceptable accuracy for practical applications.

The exhaustive literature review that we have been conducting on gas explosions shows that the CFD modelers take two different approaches to solve a reactive flow problem:

- microscopic modeling,
- macroscopic modeling.

In the microscopic modeling approach, the effort is to resolve extremely small-scale features associated with an explosion. An example of such modeling is shown in Figure 1 where the mechanics of deflagration-to-detonation transition (DDT) through the Zeldovich reaction gradient mechanism was investigated by Oran and Gamezo [3]. The microscopic modeling is normally used to explain phenomena on a more elementary level. Since the resolution scales involved in a reactive flow problems differ by several orders of magnitude, the microscopic modeling approach is severely restricted to small-scale problems. Of course, because of its more “first-principle” based approach, the confidence in the microscopic modeling results will generally be higher.

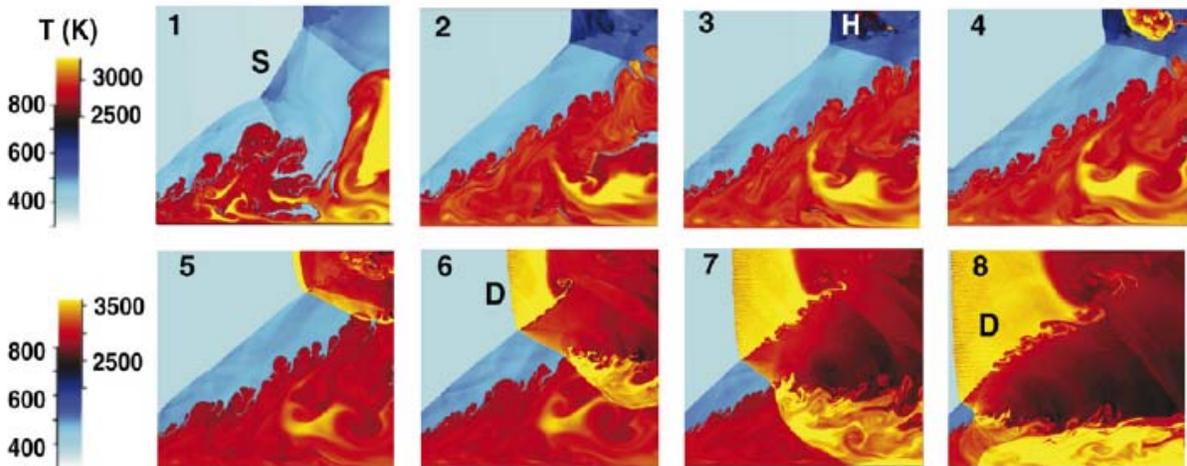


Figure 1. Temperature distribution as an explosion transitions into detonation.

In contrast, the macroscopic modeling is the most predominant method used to solve practical reactive flow problems. In this approach, simulations are made to resolve macroscopic features while including as many fundamental processes as practically possible. Since these models do not solve the problem at the most basic level, data is necessary to “calibrate” the models before they could be used for prediction purposes.

The modeling approach used for a particular problem depends on the capabilities of the CFD program used, the available computing resources and project economics. While theoretically it should be possible to model any reactive flow problem with the microscopic approach, the required computer resources are so enormous that such modeling becomes prohibitive for simulating mine-scale problems. In fact, even for medium-size reactive flow problems, microscopic modeling is simply not within the reach of many users, excluding a few government organizations.

The modeling approach adopted in the Corps' Sago report was the macroscopic one. It is important to realize that for solving the panel-scale Sago models, even the macroscopic modeling required enormous computing resources [1]. In connection with the macroscopic CFD models for reactive flow problems, Vasil'ev [4] notes,

“An initial domain with a temperature higher than the initial value is normally set in modeling ignition of the mixture; to reduce the computation time for the process dynamics, this temperature is chosen to be fairly high (often equal to a half of the temperature of the combustion products, which is several times the ignition temperature). At such high temperature gradients, expansion of combustion products from the very beginning leads to formation of compression waves of noticeable amplitudes. In computations, the amplification dynamics is most often replaced by an instantaneous explosion of certain volume of the combustible mixture, which leads to rapid formation of a DW [*detonation wave*]. The apparent solution of the DDT [*deflagration-to-detonation transition*] problem has nothing to do with real physical mechanisms of flame acceleration (autoturbulization of the combustion front, transition from laminar to turbulent burning, amplification of compression waves, and shock-wave and combustion-front instability).” *Italics added.*

The above quote indicates that several approximations become necessary in the macroscopic modeling, which may not be supported by the real processes but are introduced to simplify the solution process. The effect of such approximations is hard to assess, especially, for an area as new as coal mine explosion simulation.

Of course, we do not fully know the kind of approximations made in the numerical solution procedures employed in the SAGE program. Since SAGE is available only to restricted users, there is no way for common users to assess its full strengths and limitations. As a result of the limited access to the program, not many publications are available that document SAGE's applicability to reactive flow problems in a range of practical situations. On the other hand, the commercially available programs are well tested and the strengths and weaknesses of these programs are well documented in the open technical literature.

Despite the fact that the full details related to the SAGE program are not known to comment on the finer details of the modeling, we did find some major issues related to the inputs used for solving the Sago problem. We will address each one of them in the following sections.

2.1. Model Calibration

Since the CFD modeling used in the Corps' study was a macroscopic one, model calibration against some real data was necessary before it could be used for prediction purposes. The Corps' report used the data generated from explosion studies at the NIOSH's Lake Lynn experimental mine [5] and from Kuznetsov *et.al.* [6] pipe tests. The Lake Lynn experiments involved deflagrations and used a very small volume of methane-air as compared to the mine-scale model

used for Sago. Further, the ignition energy applied in the NIOSH experiments was 2500 J as opposed to the Sago model's 2.5 J [1]. Therefore, the higher burn rates calibrated from the NIOSH's data might have played a role in having faster transition to detonation in the Corps' Sago models. We believe, however, that the probable errors in the calibrated burn rates may not be that high.

We found some major issues in using the Kuznetsov's pipe test data for calibration, however. This Russian data was the only information that was used to check SAGE's ability to simulate the deflagration-to-detonation transition (DDT) mechanism. Before we proceed further and to clarify our reservations on using Kuznetsov's data for model calibration, it is important to understand the mechanisms involved in explosion studies conducted in obstacle-laden structures.

In a majority of the accidental gas explosions in chemical plants, offshore modules etc, some obstacles are normally present in the path of the explosion. Therefore, several studies were conducted in obstacle-laden structures to understand the explosion processes in such geometries. The presence of obstacles in the path of an explosion accelerates the burn rate and in some cases the explosion may even transition into a detonation [7]. Given sufficient length of the test pipe, it was also found that in obstacle-filled tests, the flame speed will reach a steady state after an initial accelerating phase [7]. Based on a large number of tests, four distinct explosion propagating regimes were observed in obstacle-filled pipes [7,8,9,10]:

- slow deflagration,
- fast deflagration,
- quasi-detonation, and
- detonation.

The differentiating factor among the four regimes is the speed of the flame front. For slow deflagrations, the flame speed is less than the speed of sound in unburned gas, where as it is supersonic for fast deflagration with a maximum velocity equal to the speed of sound in the combustion products [9]. Similarly, the propagating velocity lies between the Chapman-Jouget (CJ) detonation velocity and half the CJ value for a quasi-detonation. For a detonation, the propagation velocity is exactly equal to the CJ value [9]. The laboratory experiments clearly show that the transition from one regime to another is pretty drastic and clearly identifiable for certain obstacle configurations [9].

Based on several laboratory tests, Lee et. al. [7] developed a criterion to identify the conditions under which a deflagration-to-detonation transition will occur in obstacle-filled pipes. Their criterion requires that the ratio of the diameter of the orifice opening (d) and the detonation cell size (λ) of the gaseous mixture must be in the range $1 \leq d/\lambda \leq 13$. Within these limiting d/λ ratios, a quasi-detonation or a detonation can occur. It must be emphasized, however, that the d/λ criterion is a necessary but not a sufficient condition for DDT [7, 9].

Research on the explosions in obstacle-filled structures also show that despite the high flame speeds recorded for the fast deflagration regime, the measured pressures were only close to the

values estimated under constant volume adiabatic conditions. For instance, data obtained by Chao and Lee [9] for stoichiometric methane-air mixture when propagating under fast deflagration regime is shown in Figure 2. When it comes to quasi-detonation regime, Chao and Lee [9] also measured pressures that are close to constant volume estimates as shown in Figure 3.

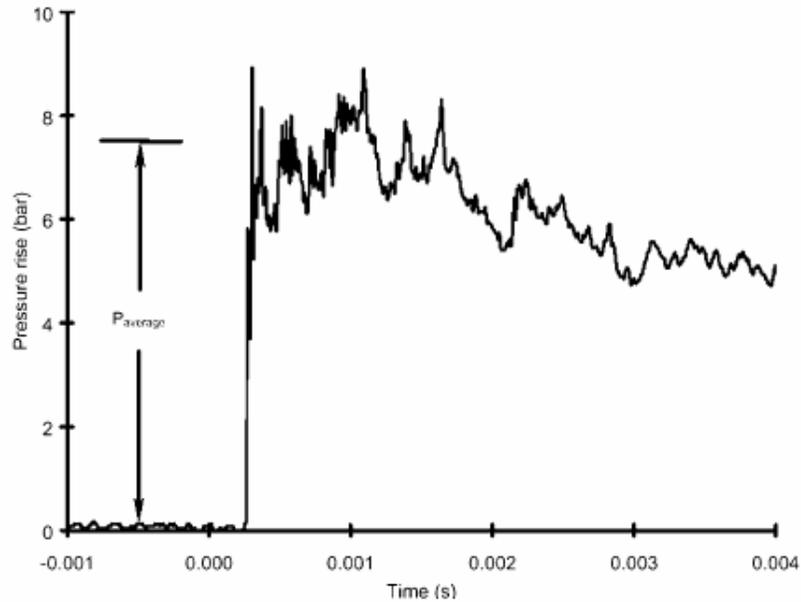


Figure 2. Pressure-time curve for a stoichiometric methane-air mix propagating under fast deflagration regime in a pipe with a blockage ratio of 0.41.

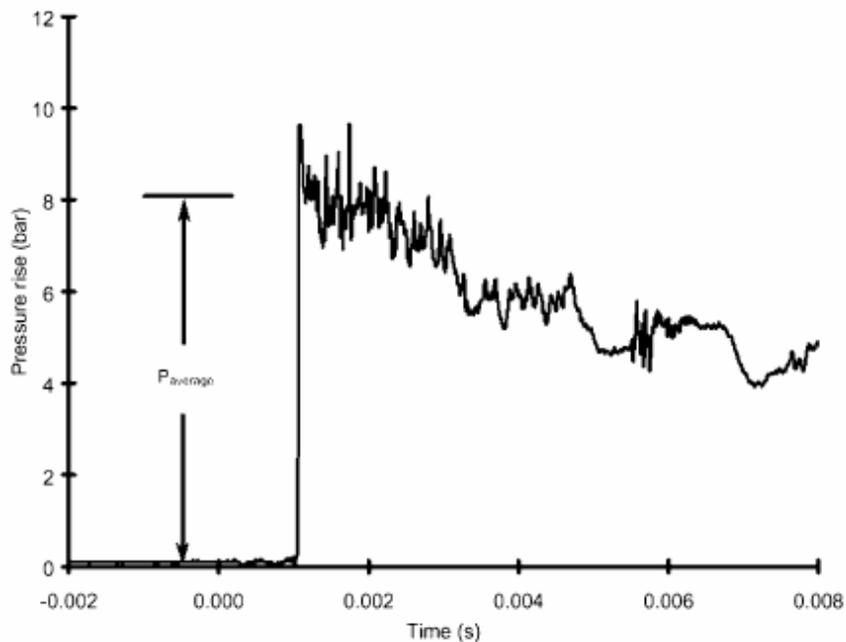


Figure 3. Pressure-time curve for a stoichiometric propane-air mix propagating under Quasi-detonation regime in a pipe with a blockage ratio of 0.41.

Further data was provided by Bjerketvedt et.al. [11] as shown in Figure 4. This later data also shows that in a fast deflagration regime, the maximum pressure reached does not exceed that estimated assuming constant volume combustion.

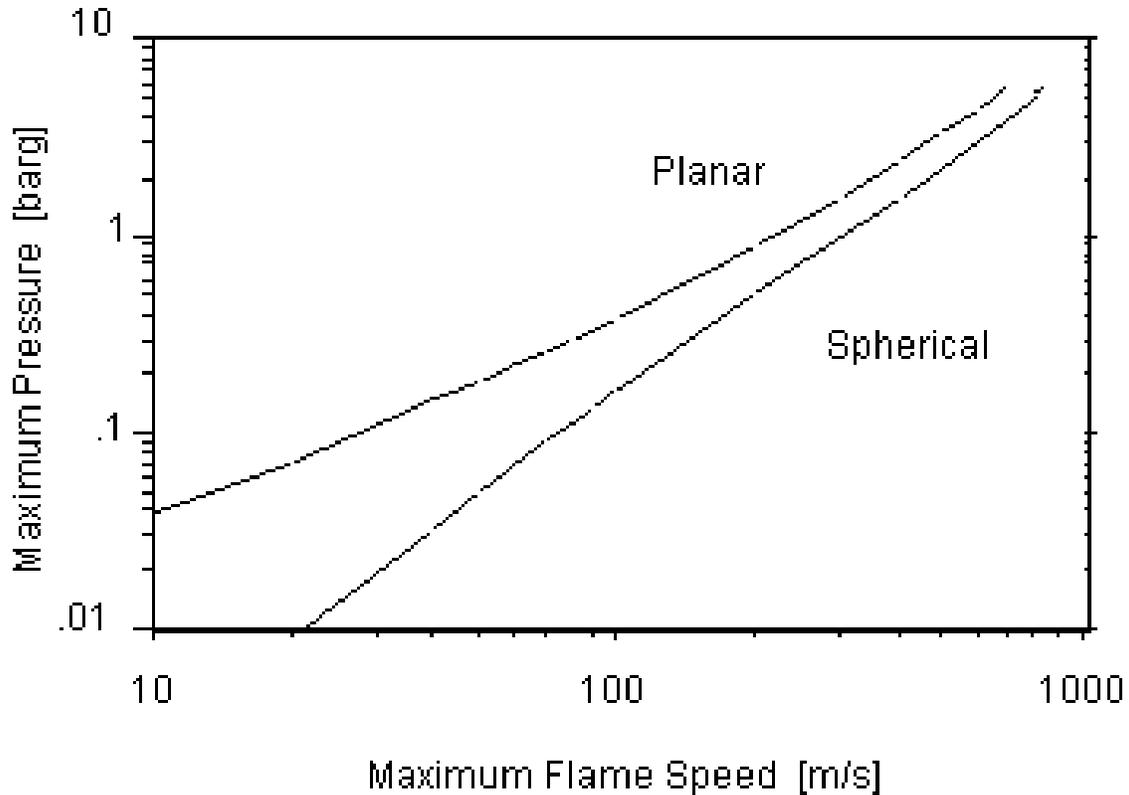


Figure 4. Peak pressure as a function of flame speed.

Research on explosions in obstacle-filled structures show that the following geometric factors will also influence the propagation regime [7,8,9,10,11,12]:

- Blockage ratio (ratio of area of obstruction to the area of the pipe),
- Obstacle shape,
- Obstacle configuration,
- Nature of the obstacle surface,
- Shape of the pipe,
- Length of pipe filled with obstacles,
- Pipe boundary conditions.

Several interesting results that show the effect of different geometries of the obstacle-filled structures on explosion output were provided by Bjerketvedt et.al. [11] as shown in Figure 5 through Figure 9.

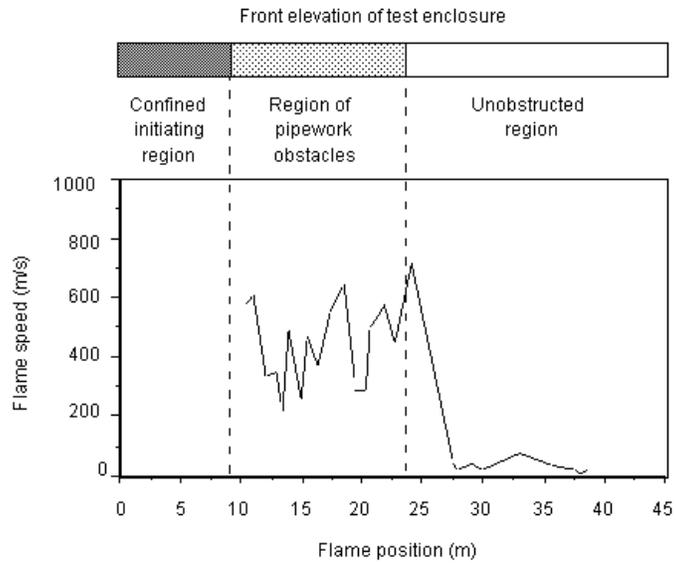


Figure 5. Change in flame speed as it passes through different regions of an obstacle-filled tube.

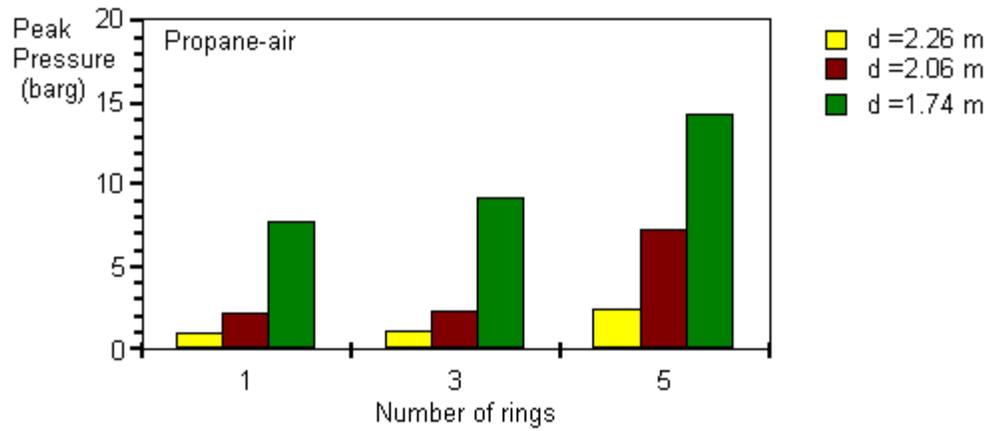


Figure 6. Change in peak pressure as a function of number of orifice plates and their size.

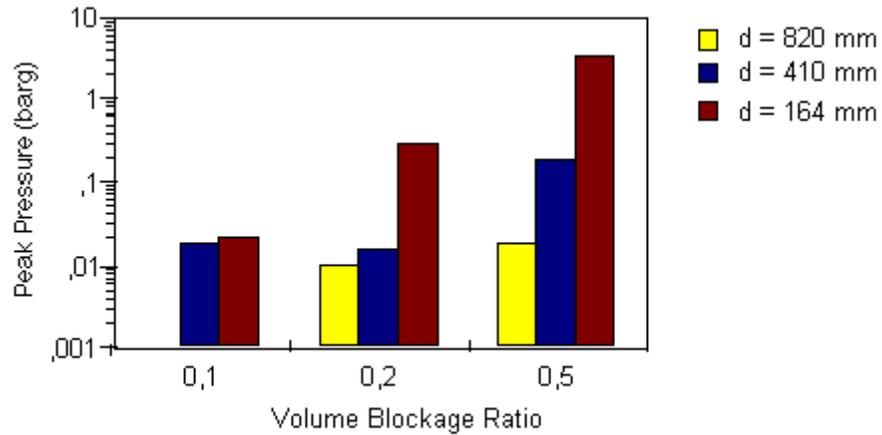


Figure 7. Change in peak pressure as a function of number of blockage ratio and the size of cylindrical obstacles in a cubical explosion vessel.

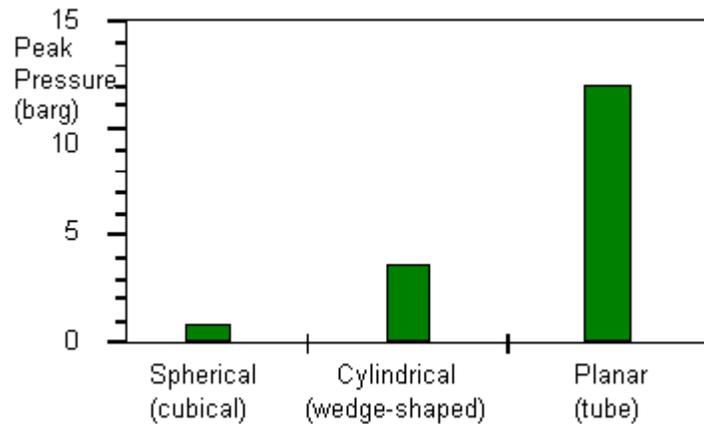


Figure 8. Change in peak pressure as a function of the explosion vessel shape for similar blockage ration in stoichiometric Propane-air mixture.

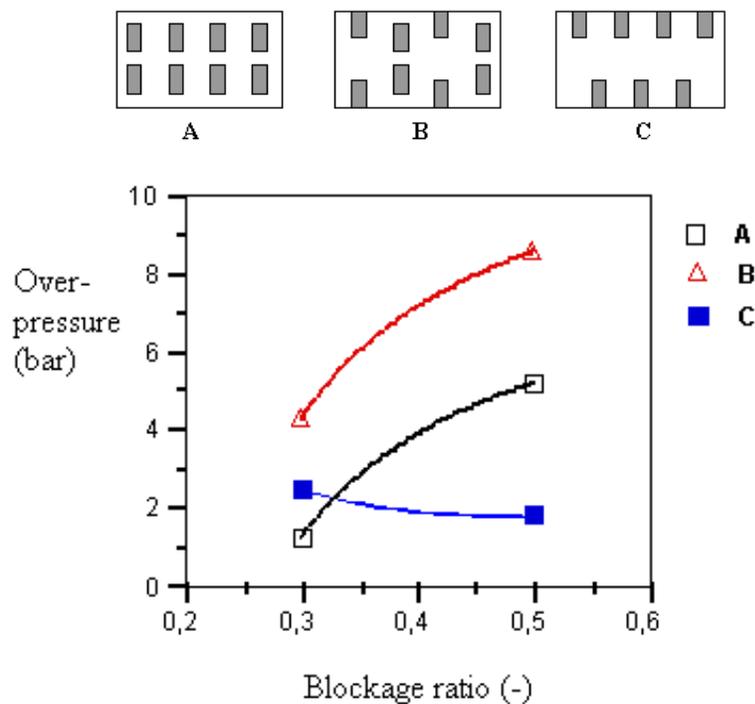


Figure 9. Change in peak pressure as a function of the obstacle configuration.

The whole point of the above discussion is to illustrate to the mining community that the results obtained in an obstacle-filled geometry are highly sensitive to the test geometry used. Also, the results obtained in a particular geometry are most likely to be unique to that geometry. Further, the obstacles must be arranged in a certain fashion to obtain a particular explosion propagation regime. Therefore, a geometry that produced quasi-detonation for a certain composition of reactive gases may not produce the same propagation regime for a difference composition of the same reactive gas.

Coming back to the Kuznetsov's pipe tests [6] used in the Corps' report for calibration, we

reproduce the following quote from Chao and Lee's paper [9] as they explain the mechanics related to orifice plate filled pipe tests very well:

"A tube filled with periodically spaced orifice plates is, essentially, a series of interconnected vented explosion chambers. As the mixture in one chamber reacts rapidly and explodes, the abrupt pressure rise can choke the flow at the orifice. The subsequent venting of the combustion products at the local sound speed produces sonic jet into the downstream chamber. The combustion front gets convected along with the jet and propagates accordingly at the local sound speed of the combustion products. This mechanism is the basis of defining so-called "choking" regime. It is clear that the propagation velocities in this regime do not accurately represent actual turbulent burning rates of high speed turbulent deflagrations. Therefore, any fluctuation from obstacle to obstacle does not accurately represent the actual fluctuations associated with an intense turbulent combustion zone."

Chao and Lee [9] also report some test results for methane-air mixtures tested in an obstacle-filled pipe. Although the pipe diameter used in these tests was smaller than the detonation cell size for stoichiometric methane-air mix, they could still measure flame speeds in excess of 1000 m/s. Based on these results, they inferred that the flame propagation in those tests was due to rapid gasdynamic expansion of the combustion products [9]. Chao and Lee's tests [9] also showed that the flame front in methane-air tests exhibited extreme fluctuations with amplitudes as large as 1000 m/s. Further, they note that:

"The fluctuations in the local velocity exhibit irregular periods of oscillation, indicating that the fluctuations do not arise from the perturbations generated by regularly spaced obstacle. Instead, the local quenching and the subsequent re-ignition of unburned gas pockets downstream is more likely to occur due to the slow kinetics of methane-air mixtures."

"Since methane-air is much less sensitive to shock induced auto-ignition than propane-air due to its long induction time, the fact that it can support the propagation of supersonic-combustion waves can not be explained in terms of shock-induced auto-ignition."

"...which strongly supports the postulate that auto-ignition of these high speed turbulent deflagrations is achieved via rapid turbulent mixing rather than by shock heating."

In contrast to Chao and Lee's tests [9], Kuznetsov et. al. [6] used a larger tube and thus they could observe the generation of quasi-detonations for a blockage ratio of 0.3. However, even in these Russian tests [6] the presence of quasi-detonation regime was strongly dependent on the gas composition as shown in Figure 10. In both the quasi-detonation regime and fast deflagration regime shown in Figure 10, the flame velocity stabilized after about 15m from the ignition point.

Considering all the complexities summarized above, it is doubtful if all the phenomena noticed in obstacle-filled pipe tests could be reproduced without resorting to the microscopic modeling approach. If macroscopic modeling is used to simulate such tests, then the validity of the results outside the scope of the test-configurations and gas compositions used in the calibration will become highly questionable. This can be clearly seen from the SAGE calibration results provided in the Corps' report [1] which are reproduced in Figure 11.

A Comparison between Figure 10 and Figure 11 shows that the SAGE program on the whole overestimates the flame speed. We think this discrepancy is perhaps acceptable considering the complexity of the problem that we are dealing with here. The major difficulty, however, is that

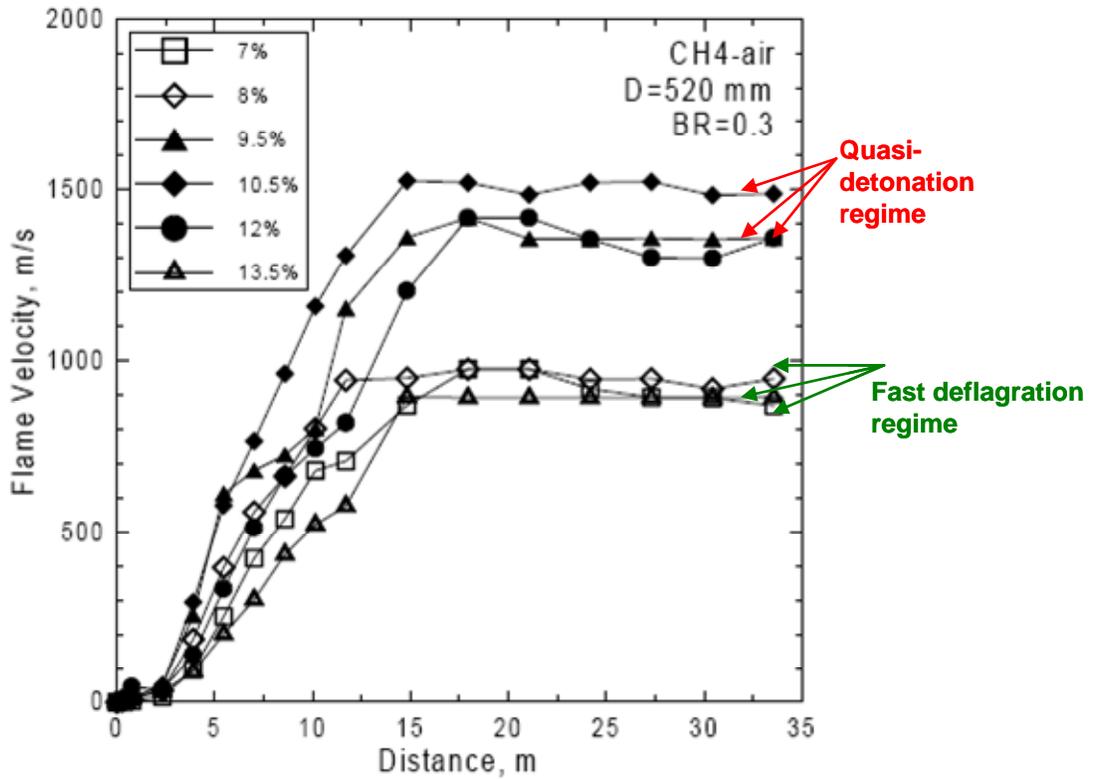


Figure 10. Change in explosion propagation regime with CH₄ composition for the Russian pipe tests used in the Corps' report.

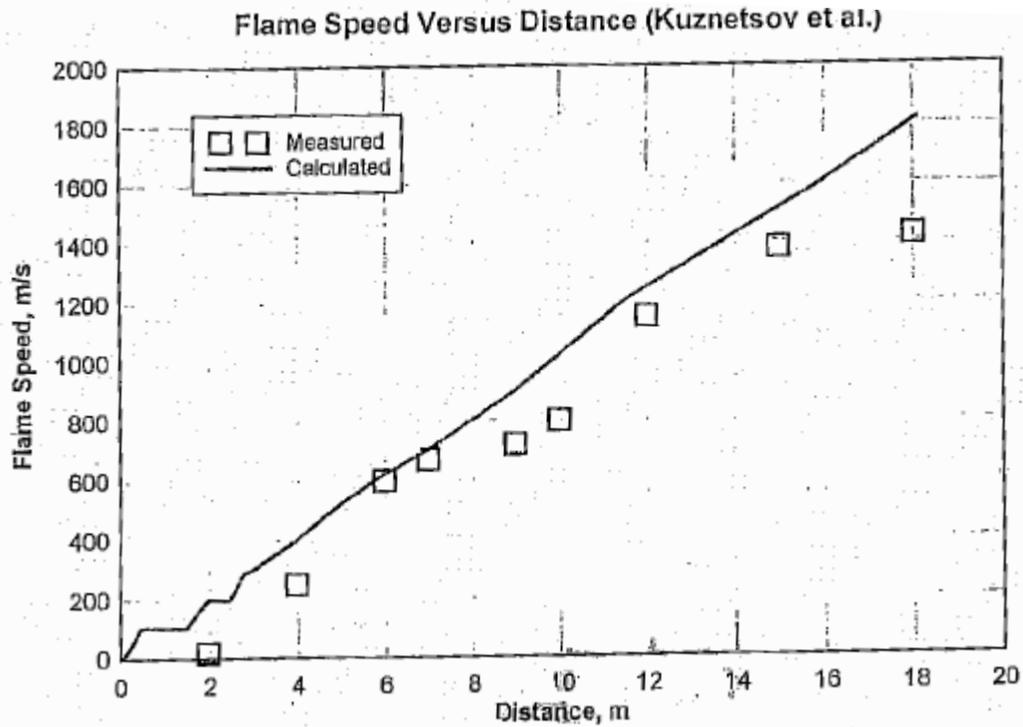


Figure II. SAGE program predicted results compared to the Russian data.

the SAGE predictions did not reach the steady-state velocity measured in the Russian tests. Looking at Figure 10, one can see that the quasi-detonation flame speed was about 1500 m/s for 9.5% CH₄. However, the SAGE predictions kept on increasing beyond the lab measured sub-CJ values and will most likely reach steady-state at the theoretical CJ value of about 1800 m/s. What this essentially shows is that the macroscopic approach used in the Corps' report has not been able to capture the complex mechanisms occurring in the obstacle-filled tubes as discussed above. As a result, the SAGE predictions will simply predict Chapman-Jouget type detonation for the Russian pipe tests, while in reality such levels were not reached. One reason for the discrepancy with the lab tests could be the lack of an explicit turbulence model and ignoring the viscous effects in the SAGE simulations.

Based on all the discussions in this section, we conclude that the calibration done for using the SAGE program to predict explosion loads at Sago was not totally accurate. The macroscopic modeling approach used in the Corps' study could not capture the mechanisms occurring in the obstacle-filled pipe tests conducted by Kuznetsov et. al. [6].

In an underground coal mine, considering the realistic gob atmosphere as discussed later in section 2.2, we believe that fast deflagrations are the most probable worst-case propagation regimes that can occur. This can be clearly seen from the Russian pipe tests shown in Figure 10 when CH₄ is outside the limits of 9.5% and 12%. Similar results on fast deflagrations in methane-air mixtures can be found in Kuznetsov et. al [13]. Of course, for the Russian tests, the remaining gases were assumed to be those of standard air. As will be seen in the next section, such a gob composition simply does not exist in real coal mine data.

Although the constant volume conditions do not exist in an underground coal mine, the explosion pressures estimated through such assumptions form the upper limit for the loads experienced under a fast deflagration regime. Therefore, we believe that the 120 psi value proposed in the ETS [14] is sufficient for design purposes. We also point out that the 120 psi load prescribed by the ETS is the highest design criterion for seals among all the coal producing countries.

2.2. Atmospheric Composition of Sealed Areas

The Corps' report uses two different gob gas compositions for the Sago mine [1]. One composition corresponds to the stoichiometric methane-air mixture whereas the second uses a combination of 8% and 17% methane-air mixtures at different levels in the Sago gob. Of course, the stoichiometric gas models have no direct relation to the Sago explosion since the amount of methane estimated by the MSHA investigations requires the presence of about 11% homogeneous methane in the Sago gob. Therefore, Runs 1 and 2 in the Corps' report represent the worst-case simulations representing practically non-existing scenarios.

In order to examine the validity of the gob atmospheres assumed in the Corps' study, we have collected a large database of samples from several operating coal mines scattered all over the country. In addition to the data from our mines, four other major U.S. coal producers have contributed their information. The coal seams included in the database are given in Table 1.

From the 24 coal mines, a total of 16222 data sets were collected. Each set includes measurements on different gob gases. All the measurements in the database were taken at the seals. Since areas just inby the seals represent the most dynamic environment of the entire gob, we think it is reasonable to assume that the gob deep inside will be more inert than represented by these measurements. Out of the 16222 sets, 11964 contain gas chromatograph data. Also, gobs of different ages – from freshly sealed to several years old – were included in the database.

Table 1. Coal seams included in the database.

| Mine Number | Coal Seam |
|-------------|----------------|
| Mine 1 | Kentucky #6 |
| Mine 2 | Pittsburgh #8 |
| Mine 3 | Kentucky #9 |
| Mine 4 | Eagle |
| Mine 5 | Kentucky #9 |
| Mine 6 | Danville #7 |
| Mine 7 | Springfield #5 |
| Mine 8 | Herrin #6 |
| Mine 9 | Springfield #5 |
| Mine 10 | Herrin #6 |
| Mine 11 | I seam |
| Mine 12 | Pittsburgh #8 |
| Mine 13 | Pittsburgh #8 |
| Mine 14 | Pittsburgh #8 |
| Mine 15 | Pittsburgh #8 |
| Mine 16 | Pittsburgh #8 |
| Mine 17 | Pittsburgh #8 |
| Mine 18 | Pittsburgh #8 |
| Mine 19 | Pittsburgh #8 |
| Mine 20 | Elkhorn |
| Mine 21 | Pocahontas 3 |
| Mine 22 | Pocahontas 5 |
| Mine 23 | I seam |
| Mine 24 | B seam |

Figure 12 below shows the plot of CH₄ against O₂ measured in the gob for all the data collected. Also shown in the figure is the stoichiometric methane-oxygen point that was used in the Corps' study. The data clearly shows that the probability of finding a stoichiometric methane-air composition in the gob is zero.

To further show the trends in the data, data points that have methane between 8% and 12% are plotted in Figure 13 against oxygen content. This plot shows that the chances of finding O₂ above 14% when methane is between 8% and 12% are extremely low. In fact, out of the total database, only 19 points had O₂ above 14% when methane was between 8% and 12%, which translates to a probability of 0.0011. Based on the trends we see in this huge database, we think the chances of finding above 14% oxygen will be reduced further as more data is collected. Since the computed probability represents gob conditions close to the seals, we believe, deep inside

the gob, the probability will perhaps be zero. Of course, not a single point in the database has the stoichiometric composition.

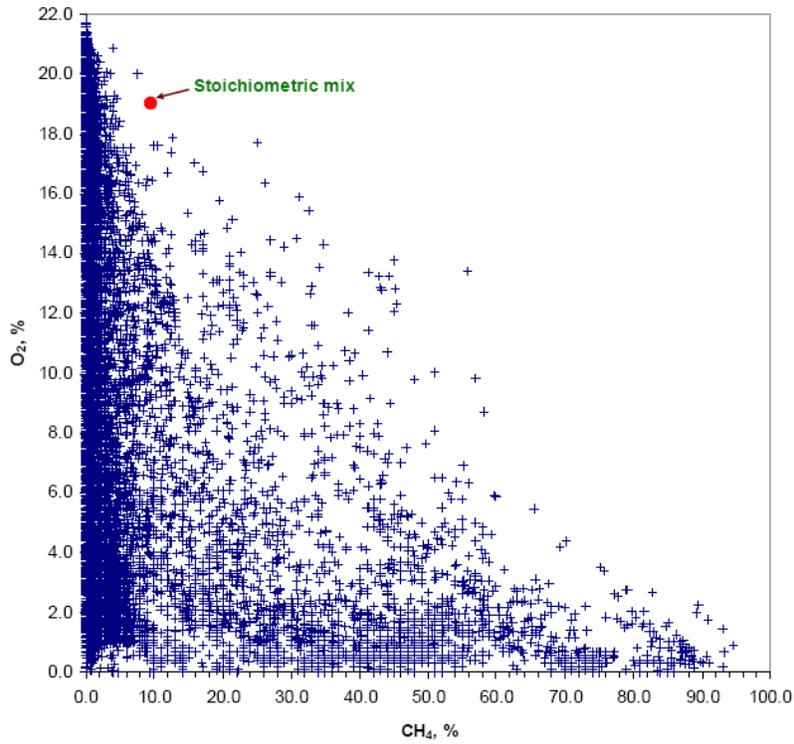


Figure 12. Methane content vs Oxygen measured for all the 16222 data points.

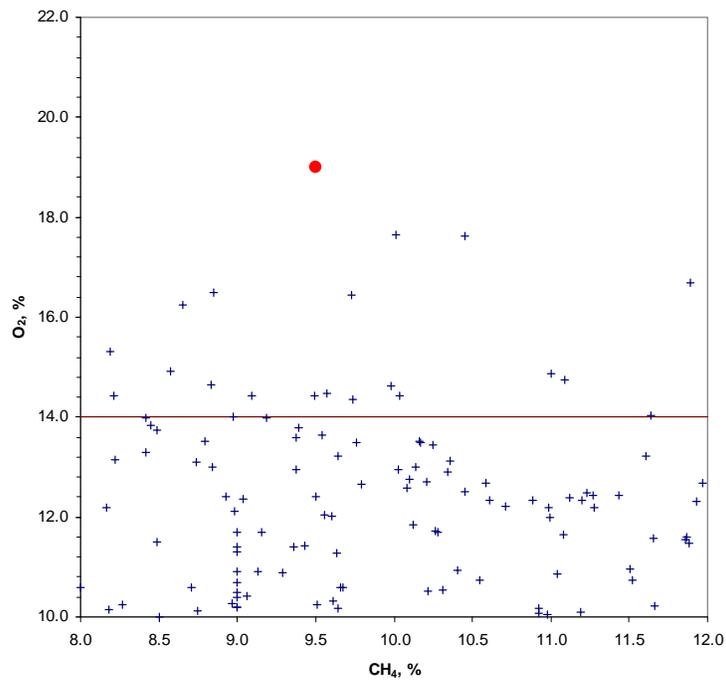


Figure 13. Measured oxygen content when methane was between 8% and 12%. (red dot corresponds to stoichiometric composition)

If one uses the Coward and Jones [15] explosibility diagram alone, then about half of the data in Figure 13 and some in Figure 12 will be considered explosive. But, from the gas chromatograph data, it was found that when methane was between 5% and 15%, a good amount of CO₂ was also detected as shown in Figure 14. Further analysis of the data shows that when methane was between 8% and 12%, the CO₂ was present in somewhat higher proportions as shown in Figure 15. Despite the presence of CO₂ and being non-explosive per the Zabetakis explosibility chart [16], for most of the cases in Figure 12 different provisions of the ETS – action plan, continuous gas monitoring etc – had to be implemented when explosiveness was assessed as described in the ETS [14].

The effect of inert gases on the explosibility has long been known and many useful studies were conducted several decades ago. Despite the availability of this wealth of knowledge, it is unfortunate that the ETS [14] relies solely on oxygen and methane contents. Based on the actual data gathered in this research, we believe that it is extremely important to consider all the gases present in a gob before deciding if it is explosive or not. In this connection, we think, it is important for MSHA to let coal mine operators use the Zabetakis explosibility diagram in addition to Coward's as a cross-check before declaring a gob as explosive and before implementing the measures required by the ETS [14].

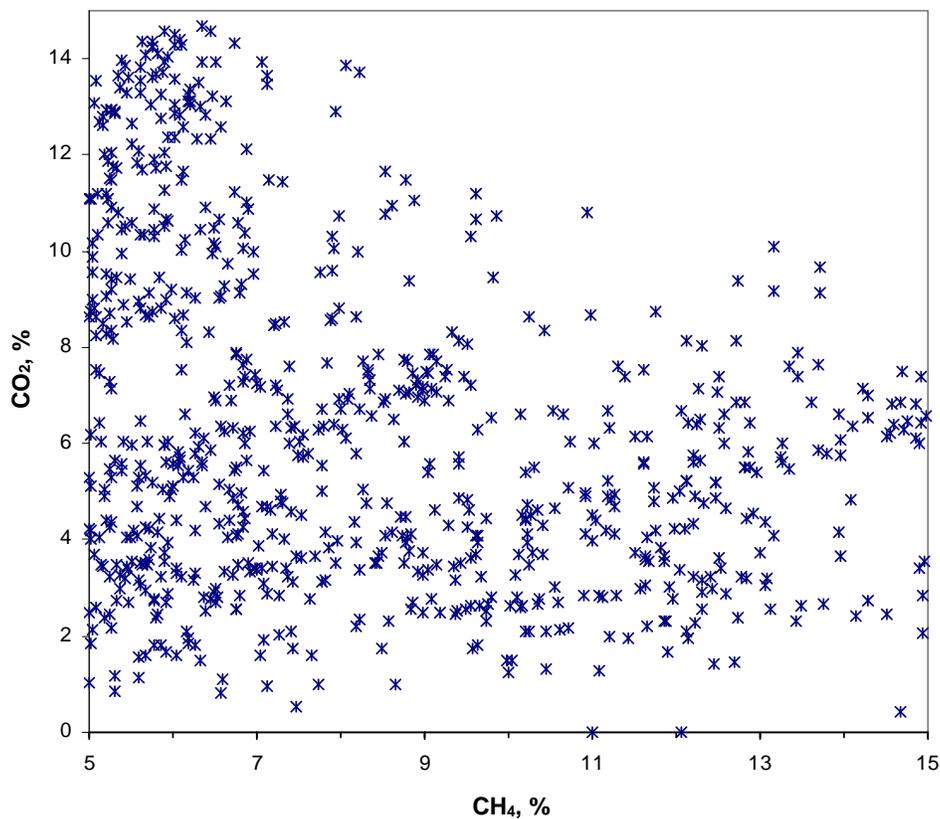


Figure 14. Measured Carbon dioxide when methane was between 5% and 15%.

The collected data also shows that the amount of Nitrogen present in the gobs is higher than that corresponding to the stoichiometric methane-air combustion. These trends are shown in Figure 16 when methane content was between 5% and 15%.

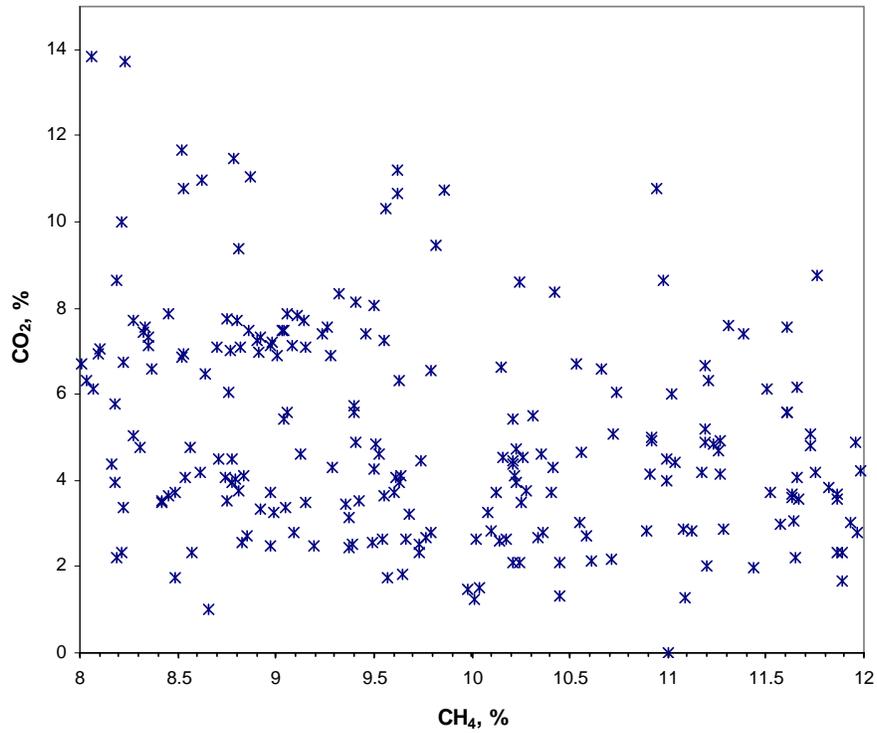


Figure 15. Measured Carbon dioxide when methane was between 8% and 12%.

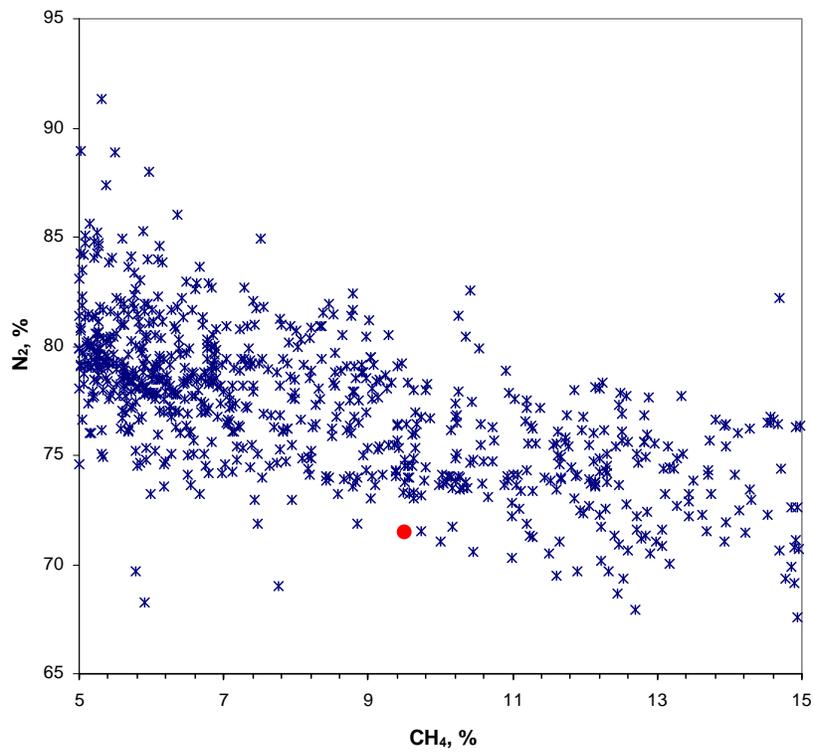


Figure 16. Measured nitrogen when methane was between 5% and 15%.
(red dot corresponds to stoichiometric composition)

As mentioned before, the Corps' study considered three different methane-air mixtures: 9.5%, 8% and 17% methane and the rest, standard air. The Corps' report assumed the 17% methane region to be inert, as it should be. The data collected as a part of this research was used to examine the composition of gob gases corresponding to the three methane levels used in the Corps' study. This data is shown in Figure 17 through Figure 19. The information in these figures clearly shows that the Corps' assumptions were not borne out by the measurements.

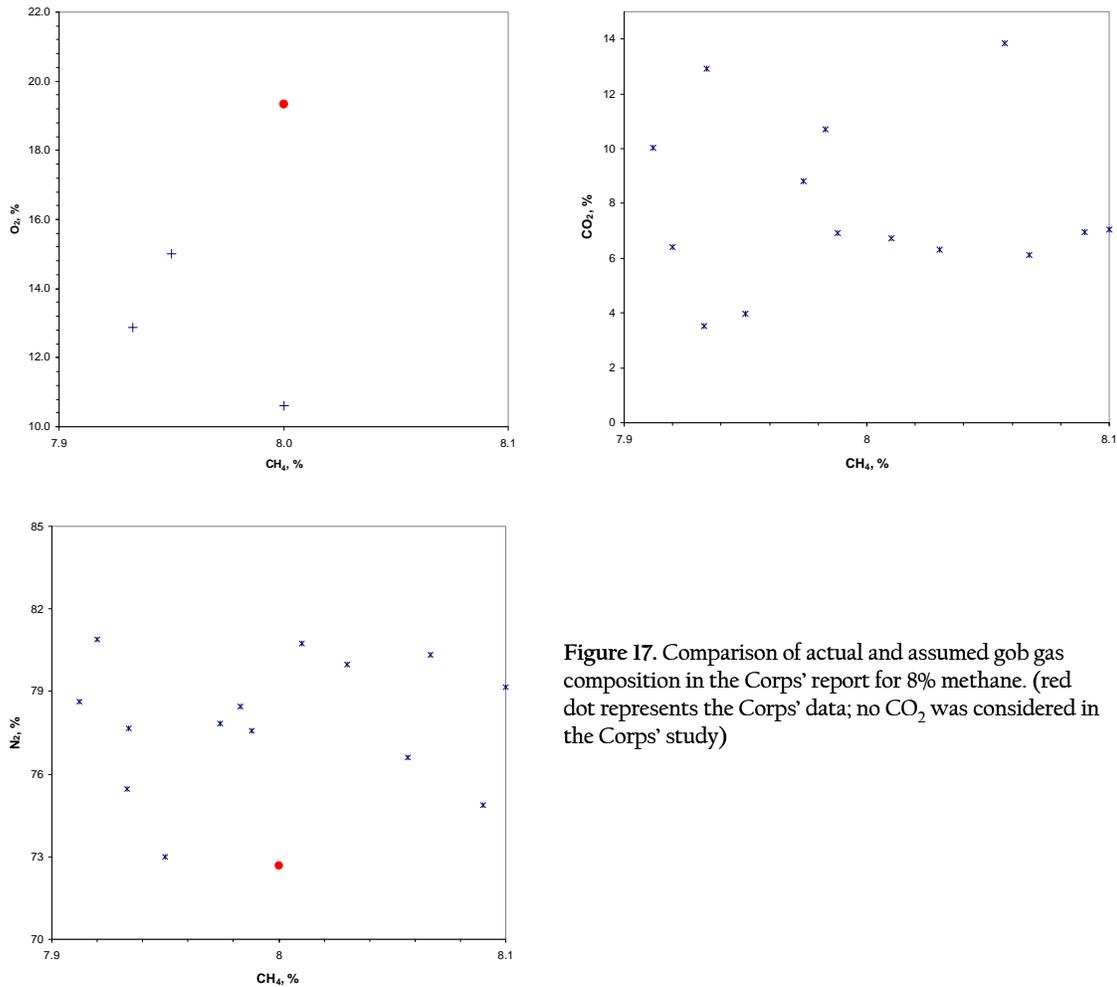


Figure 17. Comparison of actual and assumed gob gas composition in the Corps' report for 8% methane. (red dot represents the Corps' data; no CO₂ was considered in the Corps' study)

One interesting conclusion that was drawn from the data collected in this study was that the deficiency in oxygen from standard air levels was always accompanied by an increased level of carbon dioxide. This trend was noticed no matter where the coal seam was located or whether the seam was prone to spontaneous combustion or not. To illustrate the generality of this conclusion, we separated all the gas chromatograph data into two sets. In one set, data collected from Mine II in Table 1 was used to derive the relation between O₂ and CO₂ when methane was between 5% and 15% as shown in Figure 20. The best fit regression equation for the Mine II data is given by

$$CO_2 = 16.436e^{-0.1383 O_2} \quad (1)$$

The R² value for equation (1) was 0.81.

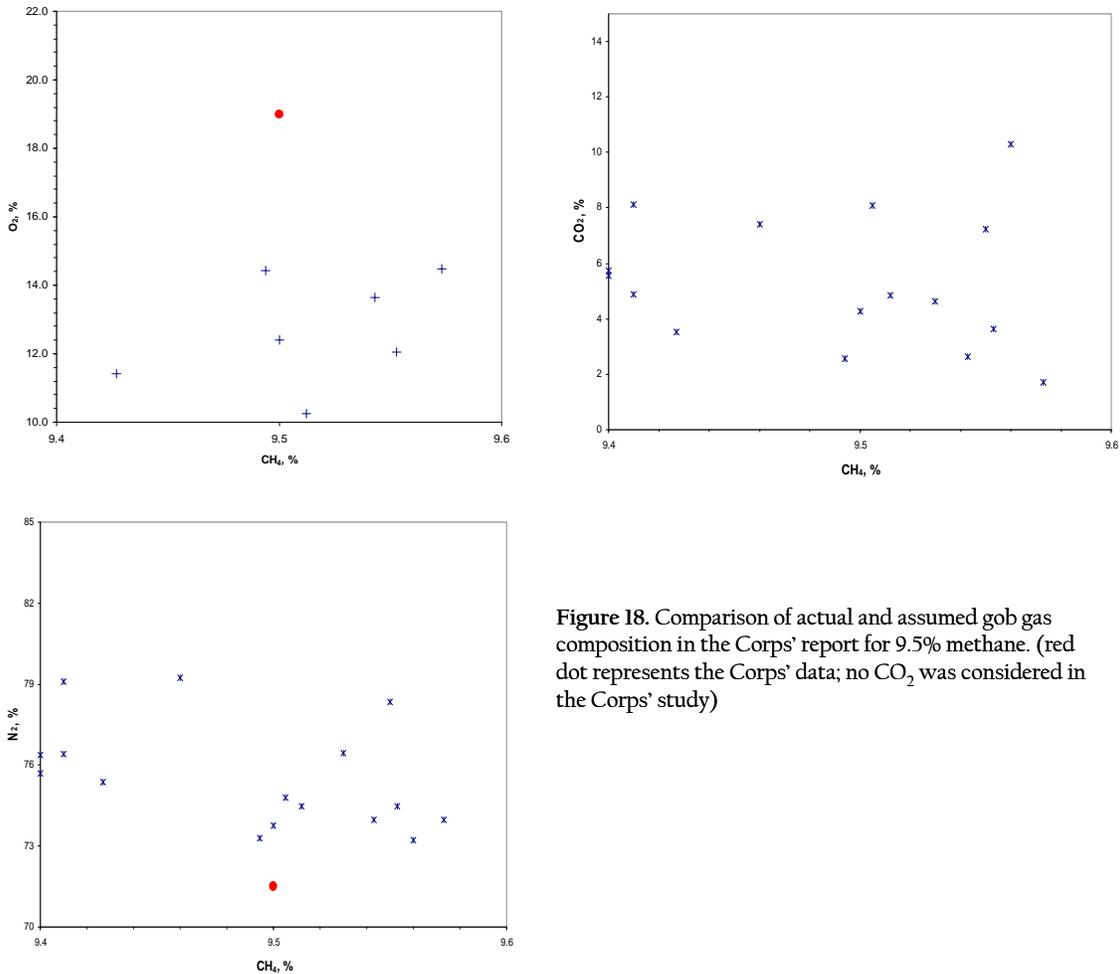


Figure 18. Comparison of actual and assumed gob gas composition in the Corps' report for 9.5% methane. (red dot represents the Corps' data; no CO₂ was considered in the Corps' study)

In the second set, data from Mine 12 through Mine 24 were combined and plotted along with equation (1) in Figure 21. If the relationship given by equation (1) is of general validity, then it should fit well for the data collected from any coal seam anywhere in the country. In fact, this assumption was borne out by the performance of equation (1) shown in Figure 21. Of course, the data in Figure 21 is more scattered than that in Figure 20. But, such a scatter is the rule rather than the exception in our field. Therefore, considering the decent performance of equation (1), it may be used to estimate the amount of CO₂ in a gob if gas chromatograph facilities or carbon dioxide samplers are not available.

An examination of Figure 12 shows that some gobs in the database measured very high amount of methane. Since a complete time-history of the gas accumulation in such gobs was not available, it may be tempting to conclude that some of those rich gobs may not follow the general trends discussed so far. While that may be a possibility, there are a few mines in the database that have shown a range of methane values because of the presence of gobs of different ages in the same coal seam. One such mine's data is plotted in Figure 22. Based on the trends shown in Figure 22, we believe that other methane rich gobs may also follow similar trends.

In summary, the huge amount of data collected from different coal seams scattered across all the major coalfields show the following trends:

- The probability of finding stoichiometric methane-air composition is zero;

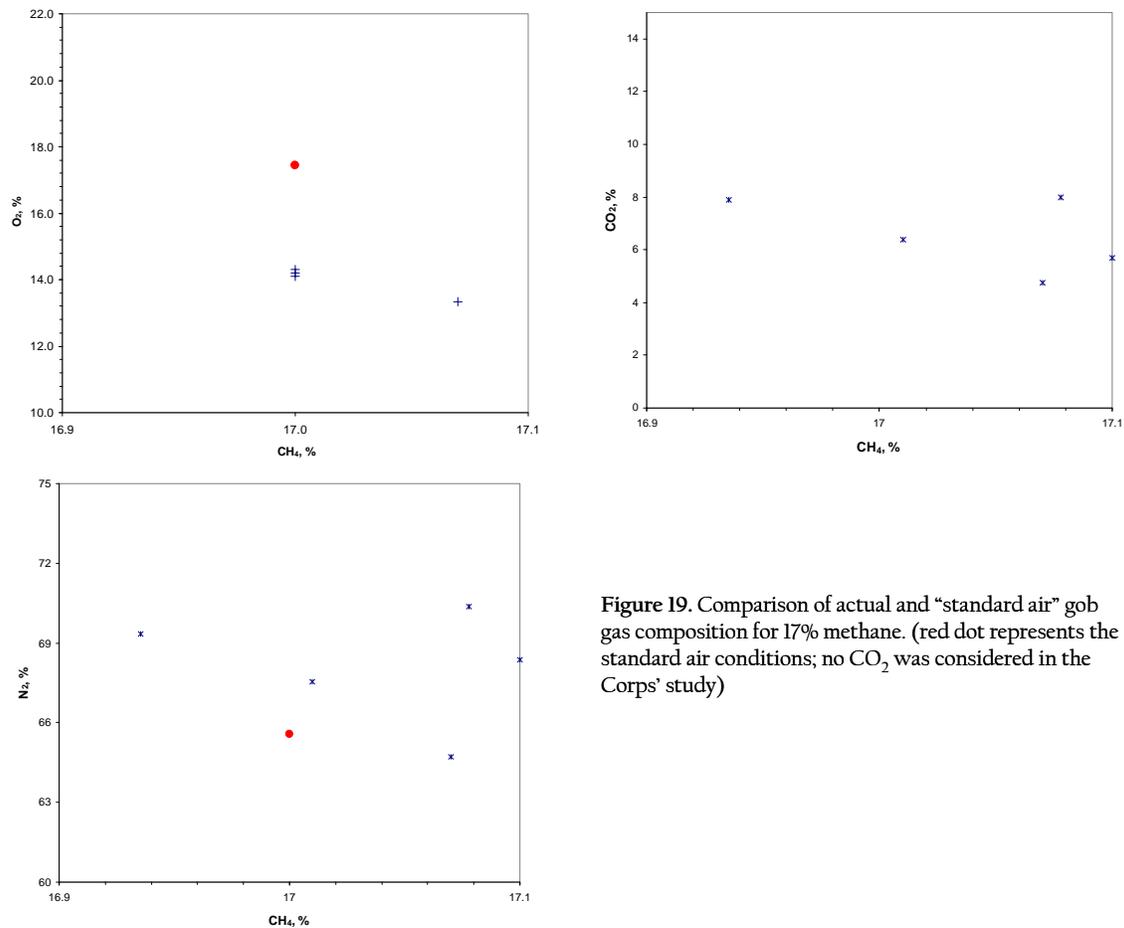


Figure 19. Comparison of actual and “standard air” gob gas composition for 17% methane. (red dot represents the standard air conditions; no CO₂ was considered in the Corps’ study)

- A more realistic upper limit for oxygen content found directly behind the seals when methane was between 8% and 12% appears to be 14%;
- Oxygen deficiency from stoichiometric levels is always accompanied by the presence of a good amount of carbon dioxide;
- Also, there is more nitrogen present in the gob than is estimated by assuming standard air conditions;
- All the gas compositions used in the Corps’ study do not exist in real gobs.

From the foregoing discussions, it is apparent that the real gobs always contain either rich or lean methane gas mixtures. Therefore, the equivalence ratio of real gob gases is either above or below 1. The implications of this type of gas composition can be seen from Figure 23, where the effect of equivalence ratio on induction length is shown [17]. The induction length is directly linked to the size of the detonation cell. Similar relation between equivalence ratio and detonation cell size is shown in Figure 24 [6,18]. The data in figures 23 and 24 clearly shows that there is a drastic increase in the detonation cell size for rich and lean mixtures compared to the stoichiometric level. It must be pointed out that the data in figures 22 and 23 corresponds to methane-air mixtures. As discussed above in this section, standard air assumption does not hold good for a real gob. Therefore, the detonation cell sizes for actual gob gases may be bigger than those predicted in Figure 23 and Figure 24. The bigger detonation cell size and the results depicted in Figure 10, clearly indicate that detonations in coal mines are highly unlikely.

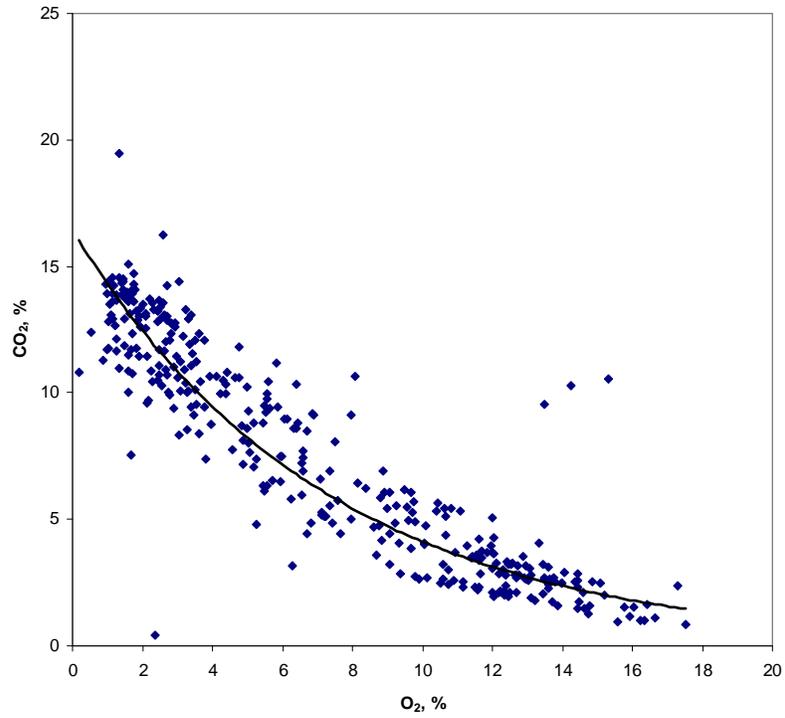


Figure 20. Relation between O₂ and CO₂ for mine 11 when methane was between 5% and 15%. Also plotted is the equation (1).

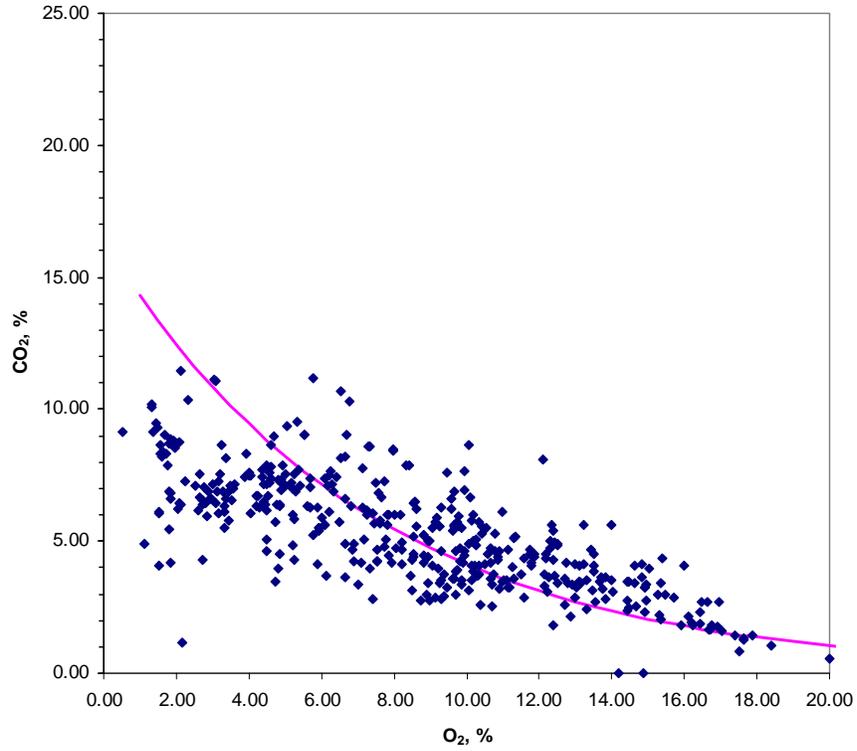


Figure 21. Relation between O₂ and CO₂ for mines 12 through 24 when methane was between 5% and 15%. Also plotted is the equation (1).

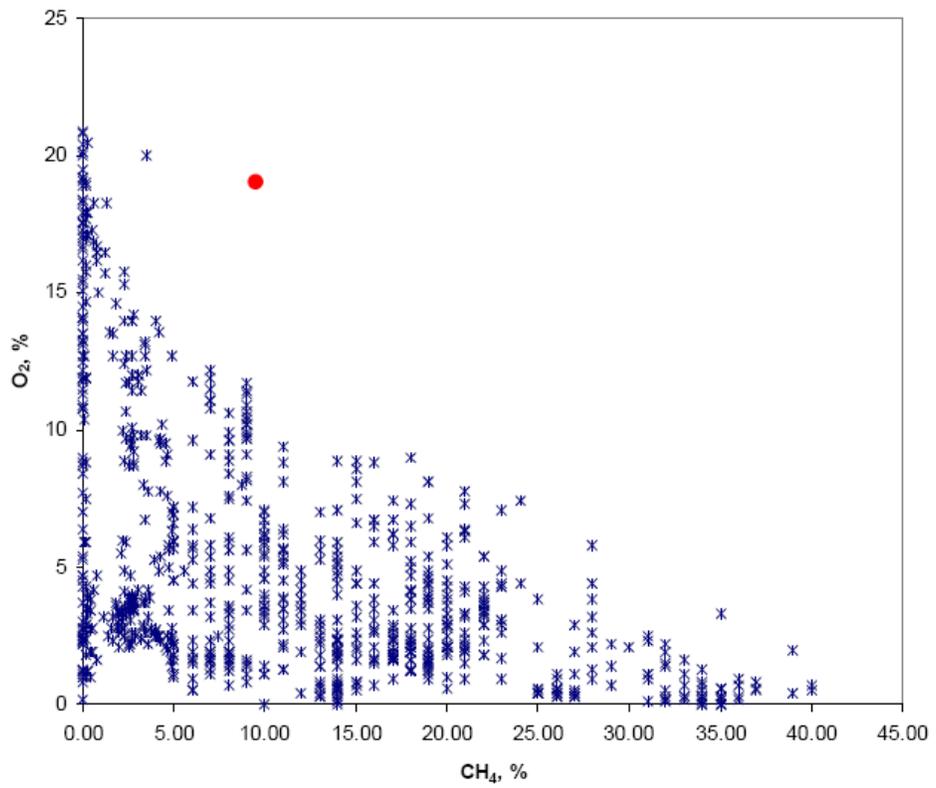


Figure 22. Relation between methane and oxygen for gobs of different ages (red dot corresponds to stoichiometric composition).

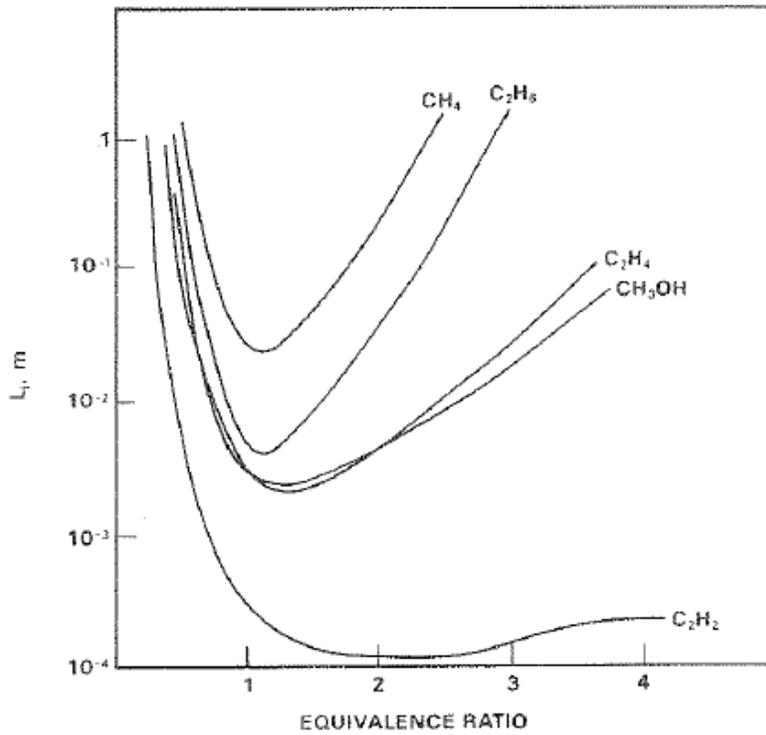


Figure 23. The effect of equivalence ratio on induction zone length for different gases.

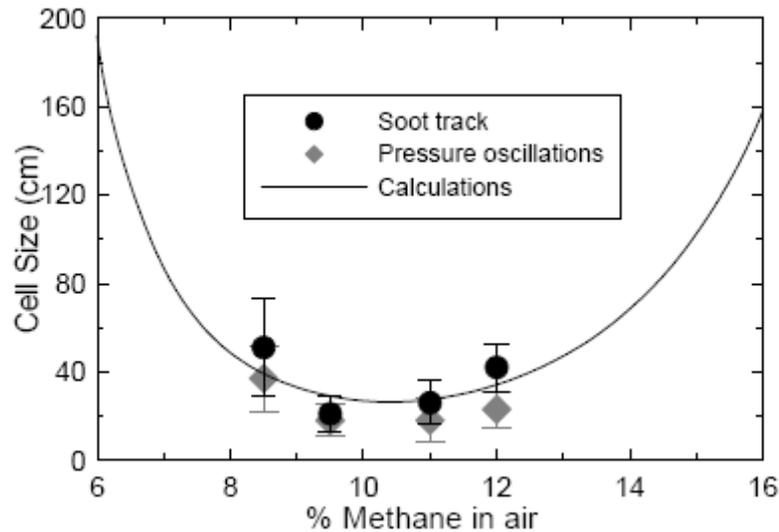


Figure 24. Change in detonation cell size with the amount of methane.

Further explanation on how a rich or lean mixture and presence of inert gases could affect explosions is very succinctly provided by Zeldovich and Kompaneets [19] as reproduced in the paragraph below:

“The shock wave amplitude, i.e., the discontinuity in pressure and temperature at which the chemical reaction is initiated and proceeds, is in turn dependent upon the detonation velocity. If we take into account the fact that the rate of the reaction depends on the temperature very strongly, then it is easy to comprehend how a small decrease in the velocity of the shock wave will be strongly pronounced in its effect on the reaction rate. However, the losses in turn increase, because during a longer time interval a larger amount of heat can be given up to the walls. The increase in the losses in turn decreases the wave velocity, and so forth. With a small reaction velocity the propagation of the detonation becomes infeasible.”

2.3. Homogeneity of Gob gases

In addition to assumptions on gas composition, the Corps’ report also assumes that a homogeneous mixture exists in the entire Sago gob in Runs 1 and 2. In Run 3, the gas was assumed to be homogeneous within each region covered by 8% and 17% methane-air mixtures. The data collected as a part of this study provided an opportunity to examine the homogeneous distribution assumption. While we do not have data for several points within the gob, some information was available to examine the nature of gas distribution on a panel scale.

Because of the location of gas sampling points around the perimeter, Mine 11 in Table 1 provided data at three corners of some longwall panels at that mine. The information was collected from two seals on the tailgate and headgate sides (seal 1 and seal 2) at the recovery room as well as from one seal on tailgate side in the bleeders at the back end of the panel (seal 3). Different gases measured at these seals over a period of time are shown in Figure 25. Data measured within a few hours on the same day were only included in Figure 25. Some more data was available from Mine 24 in Table 1, where different gob gases were measured at two seals in the headgate (HG) and tailgate (TG) of a sealed longwall panel. For the tailgate seal, the monitoring was

discontinued for some period until the ETS [14] came into existence. Therefore, data from this mine was split into two parts for different time periods as shown in Figure 26 and Figure 27.

The data in figures 25 through 27 clearly shows that the panel-scale homogeneity such as that assumed in the Corps' study does not exist in the real world. While data in these three figures gave some idea on the inhomogeneity, a complete distribution of gases can only be obtained by installing several measurement points within a gob. Such detailed studies are yet to be conducted.

The non-homogeneous distribution of gob gases can have a dramatic impact on the explosion output and its propagation. For instance, Dorofeev *et.al* [12] describe the effect of propagation of a detonation wave from a donor mixture through a gradient region to a less reactive acceptor mixture. These laboratory studies showed that if the ratio of the difference in the detonation cell size of donor and acceptor mixture and the width of the non-homogeneous gradient region exceeds a certain limit, detonations do not occur [12]. The practical implication of the results described by Dorofeev *et.al* is that if a detonation were to occur in a gob, then inhomogeneity in reactive gas distribution may quench such a detonation.

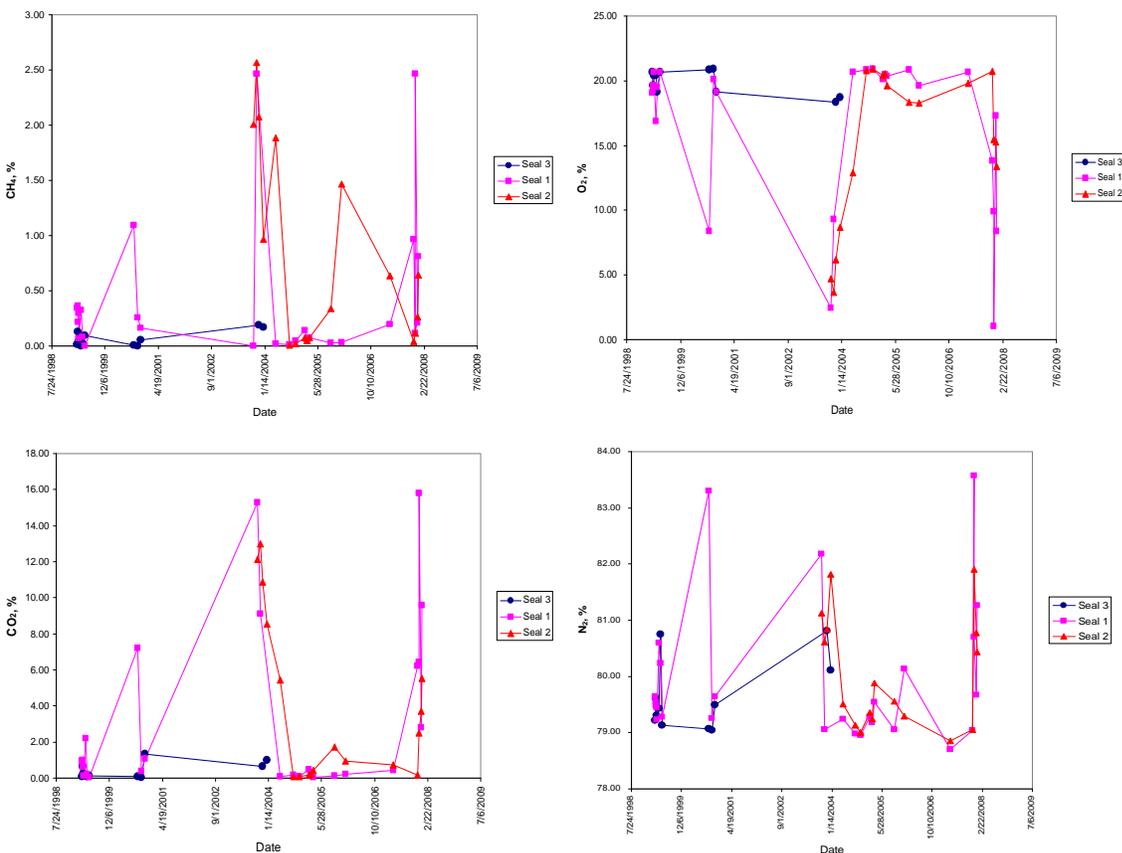


Figure 25. Distribution of different gas at three corners of a longwall panel at Mine II.

One more way that inhomogeneity will affect explosion propagation is due to the very unstable nature of the detonation front itself in hydrocarbon-air mixtures [18,20,21]. Gaseous mixtures

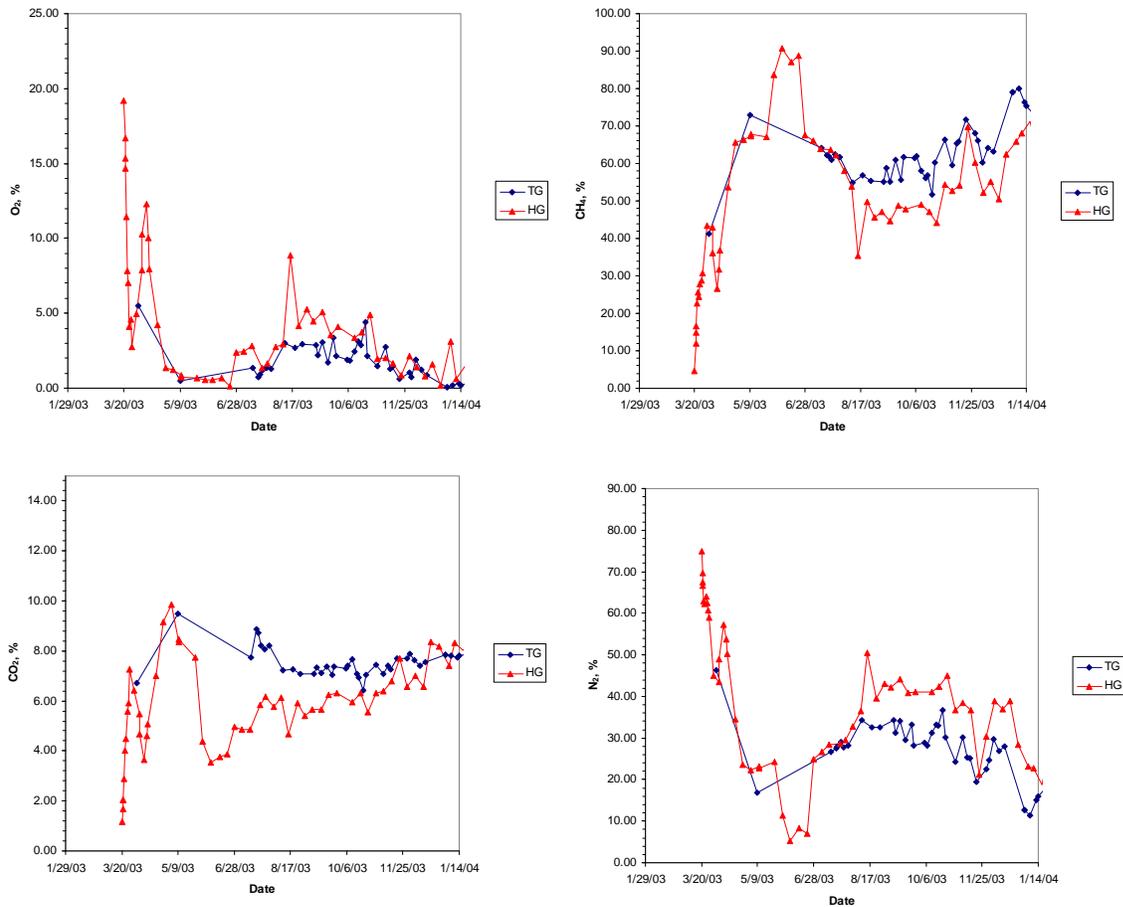


Figure 26. Distribution of different gases at the mouth of a longwall panel at Mine 24 for the earlier period.

that have high activation energy are normally associated with a very irregular detonation cell structure [21]. Such mixtures were also found to have a very unstable detonation front. Therefore, any perturbations in the homogeneity of the reactive mixture may make the already unstable detonation further unstable and may eventually result in detonation quenching.

2.4. Effect of Inert Dust

In all U.S. underground coal mines, rock dusting is done on a routine basis. This inert rock dust might influence the explosion pressures and even the propagation regimes. We have pointed out in our prior comments [22, 23] on NIOSH research [24] and on the ETS [14] that we simply can not ignore the effect of inert dust on coal mine explosions. Unfortunately, in the Corps' report also no effect of dust was considered.

When a coal mine explosion becomes a fast deflagration, the turbulence generated will blow away the inert dust placed on the excavation surfaces and suspend it in the air. Of course, some coal dust will also become suspended in the process. So, the net effect will depend on how much additional heat is added to the system by the coal dust and how much heat will be absorbed by the inert dust. The presence of dust in the reactive gas mixture changes the system composition from single-phase to a two-phase one.

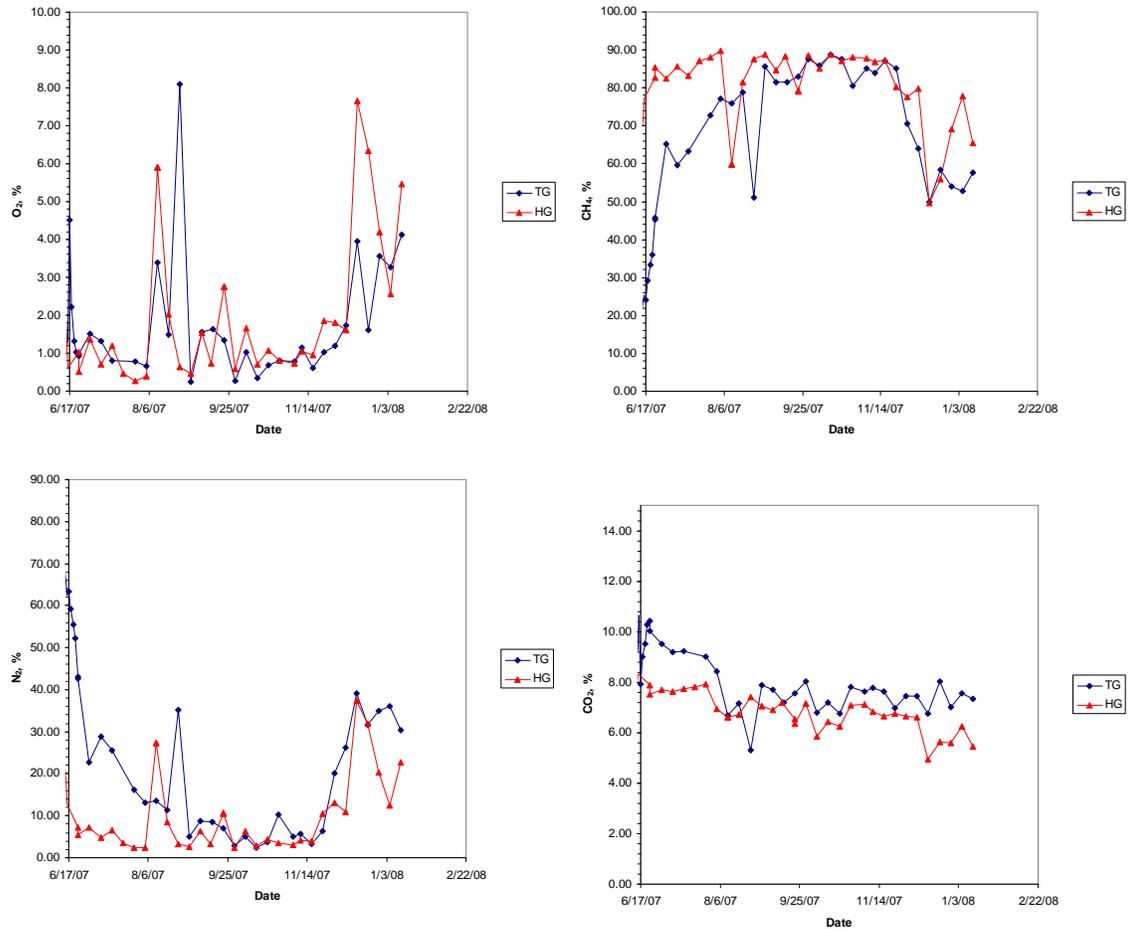


Figure 27. Distribution of different gases at the mouth of a longwall panel at Mine 24 for the later period.

The effect of suspended dust on the explosion process is much more complicated than outlined in the preceding paragraph. There are several interesting publications available on the subject in gas explosion literature [25, 26, 27, 28]. These studies show that very small inert particles under some concentrations can result in detonation quenching due to the increased energy and momentum transfer between the gas and solid phases. The multi-phase explosion studies also show that even in dilute two-phase mixtures, the inert particle concentration behind the shock front increases significantly with the propagation of the explosion resulting in the so called “compaction zone” [28].

A very illustrative study on the effect of inert dust on gas explosions was done by Papalexandris [28] using two-phase CFD modeling. These studies explain the mechanism of formation of compaction zones and the drop in the flame propagation velocities in the presence of such dense dusty compaction bands. For a particle diameter of 10^{-3} , Papalexandris studies show that when the particle volume fraction was increased from 10^{-4} to 10^{-3} , detonation quenching occurred as shown in Figure 28 and Figure 29. Of course, detonation quenching does not mean explosion suppression. Deflagration of a gaseous medium may still continue after detonation quenching.

Therefore, we believe that any realistic explosion simulation must consider the effect of dust (inert + coal) on the mode of propagation as well as on the magnitude of explosion output. For

this purpose, some physical test data must be generated with different dust concentrations and realistic gas compositions.

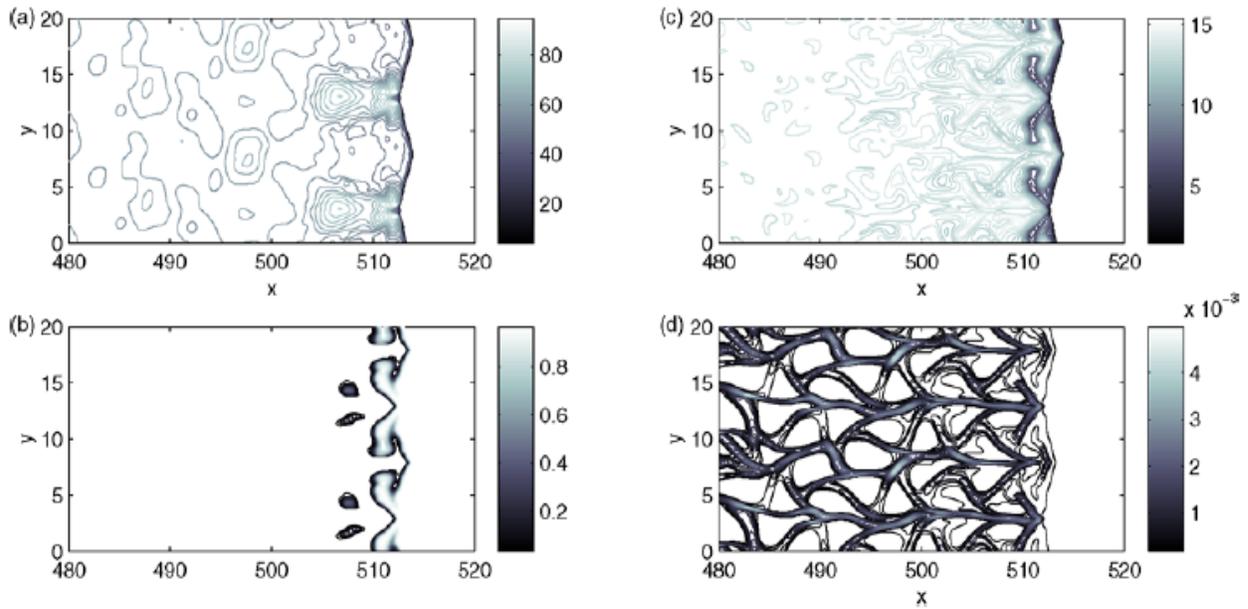


Figure 28. Distribution of (a) pressure, (b) reactant mass fraction, (c) temperature and (d) solid particle density for initial dust volume fraction of 10^{-4} .

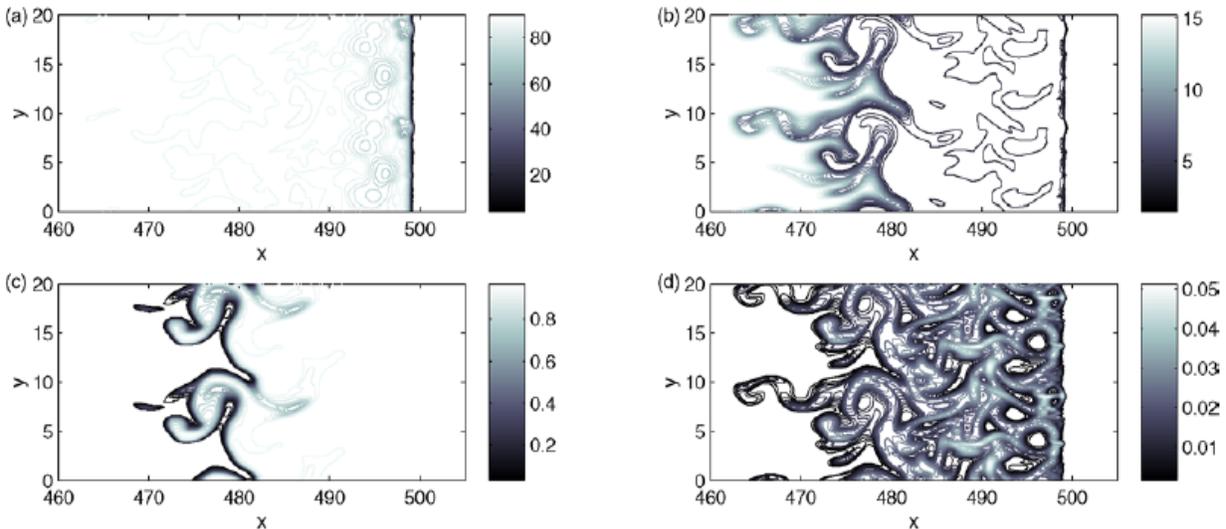


Figure 29. Distribution of (a) pressure, (b) temperature, (c) reactant mass fraction and (d) solid particle density for initial dust volume fraction of 10^{-3} . Detonation quenching can be seen in these plots.

3.0 Structural Modeling

In general, the structural modeling conducted in the Corps' report [1] was pretty exhaustive and very detailed. We do not find many issues related to the structural modeling itself. However, we have a few minor points about the inputs and the modeling philosophy as given below.

3.1. Omega Block Seals

With regard to the Omega block seal models, it appears that the Corps' report used fixed boundary conditions right on the seal boundaries itself. We think the more correct approach would be to model a good portion of the mine opening all around the seal and then apply the boundary conditions. If the boundary conditions are imposed right on the seal, then the seal becomes more stiff and can accept higher loads before failing than it can realistically deal with under extended model boundaries.

It also appears that the Omega block-to-block contacts were explicitly modeled in the Corps' report. However, nothing was given in the Corps' report as to what kind of properties were assigned to the contacts. It is also not clear from the report whether rigid or deformable contacts were used.

The final and most important objection to the seal modeling is in the selection of the constitutive model for the Omega block materials. The volumetric strain-mean stress curve used for the Omega block material in the Corps' report shows strain hardening behavior in the post-yield zone whereas the real behavior is strain-softening one as illustrated in Figure 30. The data in Figure 30 was taken from Tom Barczak's Ph.D. work on mine stoppings[29]. Further, the yield load used in the Corps' report seems to be higher than that in Figure 30.

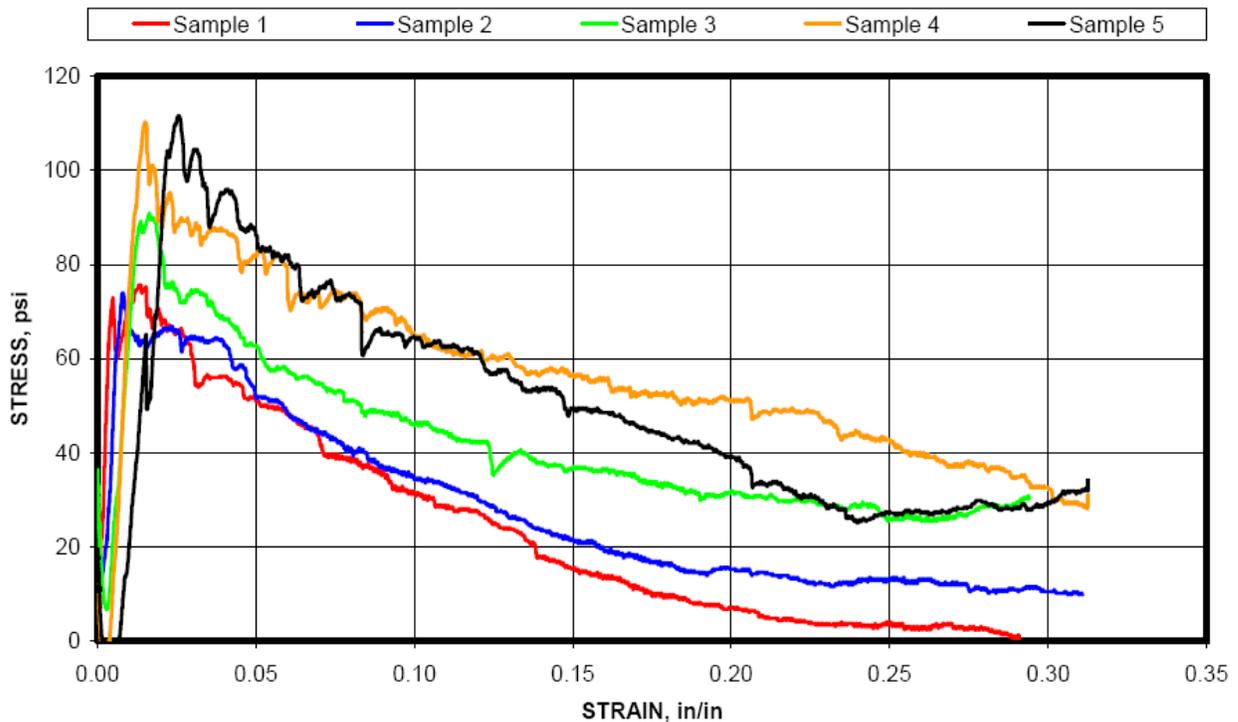


Figure 30. Axial stress – axial strain curves for 6” x 6” Omega block material.

The above three issues are minor problems and could easily be corrected by running additional models. But, the effect of the three questions raised above is to increase the capacity of the Omega seals before they fail.

It is not clear from the Corps' report, if any parametric modeling was conducted to assess the effect of different qualities of construction of the seals at Sago. MSHA's investigations [30] into the Sago explosion showed that the failed Omega block seals were not properly constructed at the mine.

Before we leave the discussion on the seal models, we would like to point out to the mining community that the seal failure shown in the Corps' report, for example, Figure 101, where the seal was shown to have been blown into little pieces was not modeled that way. It was only a visualization method that used some set criterion to plot failed elements that way. The models do not consider fracture development through intact material like that possible with discrete particle flow codes.

3.2. Belt Hangers, Roof Bolts, Spider and Pie Plates

We think the Corps' fluid-structure interaction modeling to study the effect of explosion loading on plates and bolts deserves a lot of praise. We believe the modeling approach used is very comprehensive and thorough. We, however, have a couple of minor issues related to this modeling.

Although the peak pressure front lasts only for a few milliseconds, and the dynamic pressures become equilibrated very quickly, we think the thermal degradation of the yield strength and modulus of elasticity must have been considered in the modeling. The Corps' CFD model results qualitatively show that after the passage of the first pressure wave, a few lesser magnitude spikes were noticed in the modeled pressure-time curves. The secondary spikes were due to the reflected waves or due to some other explosion fronts coming subsequent to the passage of the first wave. We think the time gap between these multiple load fronts is sufficient to increase the temperature of the modeled structures to some extent.

We believe that the final deformed geometry of the belt hangers, bolts and plates might have been reached in multiple stages with different amount of deformations produced by different wave fronts reaching the location of these structures. Despite the smaller magnitude of the secondary pressure waves, sizeable deformations of the structures are possible due to the lowered yield strength under the influence of the high temperatures generated by the primary combustion wave. Although the final temperatures were in the range of 2000°F, such high values are not necessary to reduce the yield strength to a noticeable level. This can be seen from Figure 31, where the effect of temperature on the yield strength of steel is shown [31].

We also think that the final deformations measured for belt hangers can not be used to reliably estimate the magnitude of dynamic pressures that those structures have experienced. As the Corps' report itself identified, the belt hangers could have been deformed to some extent while they were under the service loads when the area was being extracted. Also, the bolts, belt hangers and plates were in the mine for several months and it is not known if any strength loss in these materials had occurred under the action of mine water and other corrosion causing factors.

In conducting fluid-structure interaction type models for spider and pie plates, it appears that Corps' report considered some uniform gap between the roof and the plate. However, as

common observations underground show, the gap is rarely uniform. In fact, the gap between the roof and the plate decreases from the plate edge to the center. Such non-uniform gaps will require lower dynamic pressure to deform the plate because of the initial non-zero angle that the plate makes with the flow direction. Additionally, if multiple pressure waves reach a plate location, then for every subsequent wave, more plate surface is exposed to the dynamic pressures.

For all the above reasons, we believe that the dynamic pressure magnitudes required to deform belt hangers, roof bolts, pie and spider plates may have been overestimated in the Corps' study.

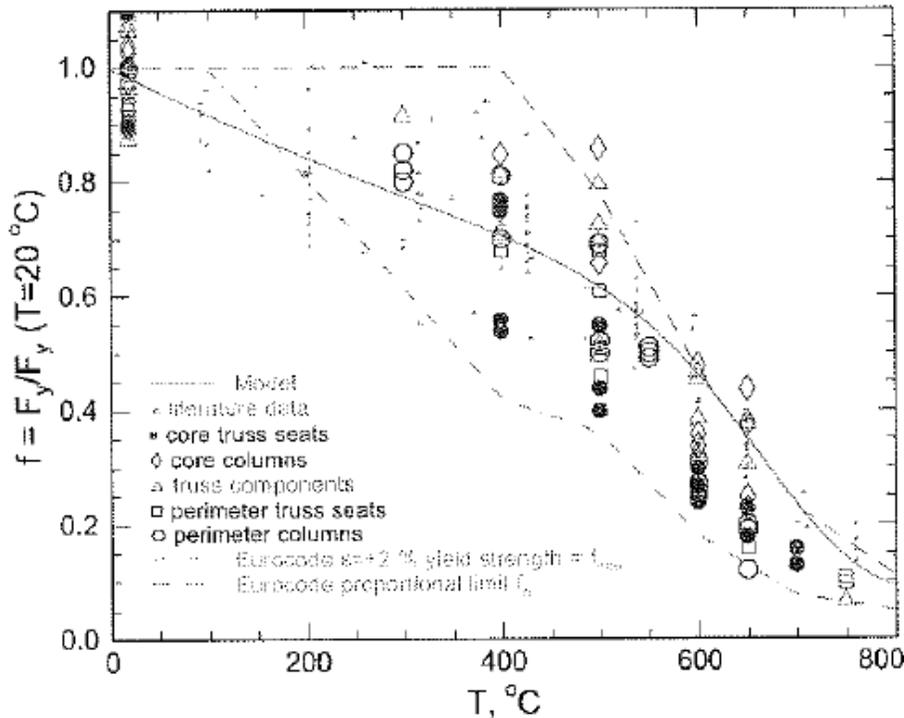


Figure 31. The effect of temperature on the yield strength of steel.

4.0 Conclusions

Based on the data and the research presented in this note, we draw the following conclusions:

- The Corps' studies on the Sago explosion were well conducted within the limitations of the inputs provided to them. However, because of the unrealistic assumptions made about the gob atmospheres, we think the Corps' study can not be used as the basis for any practical seal design purposes.
- While the CFD modeling by itself is highly sophisticated, the macroscopic modeling approach used was not reliable enough to use for prediction purposes. As discussed in this note, the mechanics of explosion propagation in obstacle-filled tubes were not properly captured by the SAGE simulations. Further, the explosion propagation mechanisms in obstacle-filled structures are not applicable to coal mine entries.

- The large amount of gob atmospheric data collected for our comments shows that the probability of finding a stoichiometric methane-air composition in a gob is zero. The data also shows that the chances of finding oxygen content greater than 14% when methane was between 8% and 12% were negligibly small.
- The data indicates that some amount of carbon dioxide is almost always present when oxygen content is below the stoichiometric level. An equation has been developed to estimate the approximate amount of CO₂ as a function of oxygen when methane content was between 5% and 15%. This equation may be used to estimate the amount of CO₂ given the oxygen content if gas chromatograph analysis is not done or if a carbon dioxide sampler is not available.
- It is unrealistic to ignore the effects of CO₂ on methane explosibility. We think MSHA must let mine operators use both Coward's and Zabetakis diagrams to assess whether a gob is explosive or not. In the absence of gas chromatograph data or CO₂ gas detectors, equation (1) given in this note may be used to estimate the carbon dioxide concentration.
- The data also shows that panel-scale homogeneity such as that assumed in the Corps' study does not exist in reality. In addition to its effect on the explosion output, the inhomogeneity also has implications towards the way MSHA is implementing "action plans" when an explosive mix is detected per the ETS. Since actual gob composition is highly non-homogeneous, we believe that MSHA should let mine operators make a risk assessment of the affected area when a single isolated measurement at some point in a coal mine is found to be explosive per Zabetakis and Coward's diagrams.
- The effect of inert dust on the mode of propagation and the magnitude of explosion output could be significant. Thus, in addition to some physical tests, two-phase modeling must be conducted to incorporate the effects of dust on explosion pressures.
- Considering the actual gob gases and the effect of inert dust and large diameter Russian pipe tests shown in Figure 10, we believe that the most realistic worst-case mode of explosion propagation in coal mines is the fast deflagration regime. Further, our analysis shows that the chance of having methane gas detonation in a coal mine is almost zero.
- Although conditions for constant volume adiabatic combustion do not exist underground, research cited in our comments indicates that such calculations form the upper limit for the fast deflagration loads. Further, using the actual gob compositions analyzed in this note, the constant volume explosion loads were found to not to exceed 100 psi. Therefore, the 120 psi criterion in the ETS has an adequate safety factor included in it.
- Some realistic laboratory and mine-scale physical tests are necessary to develop the required information for a proper calibration of the CFD models. These tests must consider the realistic gob gas compositions and the effect of dust as discussed before.
- There were a few minor issues related to the structural modeling conducted in the Corps' report. We think the effect of improper constitutive model for Omega block materials, imposing fixity conditions on the seal itself, ignoring the effect of temperature on yield strength of steel and the uncertainty of the pre-explosion state of the belt hangers, plates and roof bolts, resulted in an overestimation of the explosion pressures needed to deform those structures.

References

1. McMahon, G.W., Britt, J.R., O'Daniel, J.L., Davis, L.K., Walker, R.E. CFD Study and Structural Analysis of the Sago Mine Accident. U.S. Army Corps of Engineers, Engineer Research and Development Center, ERDC/GSL TR-06-X, Final Draft, May, 2007, 138 pp.
2. Oran, E.S., Boris, J.P. *Numerical Simulation of Reactive Flow*. Second Edition. Cambridge University Press, 2001, 529 pp.
3. Oran, E.S., Gamezo, V.N. Origins of the deflagration-to-detonation transition in gas-phase combustion. *Combustion and Flame*, 148, 2007, 4-47.
4. Vasil'ev, A. A. Estimation of Critical Conditions for the Detonation-to-Deflagration Transition. *Combustion, Explosion, and Shock Waves*, 42(2), 2006, 205-209.
5. Sapko, M.J., Weiss, E.S., Cahdollar, K.L., Zlochower, I.A. Experimental Mine and Laboratory Dust Explosion Research at NIOSH. *Journal of Loss Prevention in the Process Industries*, 13, 2000, 229-242.
6. Kuznetsov, M., Ciccarelli, G., Dorofeev, S., Alekseev, V., Yankin, Yu, Kim, T.H. DDT in methane-air mixtures. *Shock Waves*, 12, 2002, 215-220.
7. Lee, J.H., Knystautas, R., Chan, C.K. Turbulent Flame Propagation in Obstacle-Filled Tubes. Proceedings of the 20th International Symposium on Combustion, The Combustion Institute, 1984, 1663-1672.
8. Peraldi, O., Knystautas, R., Lee, J.H. Criteria for Transition to Detonation in Tubes. Proceedings of the 21st International Symposium on Combustion, The Combustion Institute, 1986, 1629-1637.
9. Chao, J., Lee, J.H.S. The propagation mechanism of high speed turbulent deflagrations. *Shock Waves*, 12, 2003, 277-289.
10. Chao, J., Kolbe, M., Lee, J.H.S. Influence of Tube and Obstacle Geometry on Turbulent Flame Acceleration and Deflagration to Detonation Transition.
11. Bjerketvedt, D., Bakke, J.R., van Wingerden, K. Gas explosion handbook. *Journal of Hazardous materials*, 52, 1997, 1-150.
12. Dorofeev, S.B., Sidorov, V.P., Kuznetsov, M.S., Matsukov, I.D., Alekseev, V.I. Effect of scale on the onset of detonations. *Shock Waves*, 10, 2000, 137-149.
13. Kuznetsov, M., Alekseev, V., Yankin Yu, Dorofeev, S. Slow and Fast Deflagrations in Hydrocarbon-Air Mixtures. *Combustion Science and Technology*, 174, 2002, 157-172.
14. Department of Labor, Mine Safety and Health Administration, Sealing of Abandoned Areas; Final Rule. Published in the Federal Register, Vol. 72, No. 98, Tuesday, May 22, 2007.
15. Coward, H.F., and Jones, G.W. Limits of flammability of gases and vapors. U.S. Department of Interior, Bureau of Mines, Bulletin 503, 1952.
16. Zabetakis, M. G. Flammability Characteristics of Combustible Gases and Vapors. Department of Interior, Bureau of Mines, Bulletin 627, 1964.
17. Nettleton, M.A. *Gaseous Detonations: Their Nature, Effects and Control*. Chapman and Hall, 1987, 255 p.
18. Gavrikov, A.I., Efimenko, A.A., Dorofeev, S.B. A Model for Detonation Cell Size Prediction from Chemical Kinetics. *Combustion and Flame*, 120, 2000, 19-33.
19. Zeldovich, Ia. B., Kompaneets, A.S. *Theory of Detonation*. Academic Press, 1960, 284p.

20. Kuznetsov, M.S., Alekseev, V.I., Dorofeev, S.B. Comparison of critical conditions for DDT in regular and irregular cellular detonation systems. *Shock Waves*, 10, 2000, pp. 217-223.
21. Shepherd, J.E. Detonation: A Look Behind the Front. 19th International Colloquium on the Dynamics of Explosions and Reactive Systems, Hakone, Japan, July 27 – August 1, 2003.
22. Gadde, M.M., Beerbower, D.A., Rusnak, J.A., Honse, J.W. Comments on the NIOSH Draft Report, “Explosion Pressure Design Criteria for New Seals in U.S. Coal Mines” submitted to the National Institute of Occupational Safety and Health, 2006.
23. Gadde, M.M., Beerbower, D.A., Rusnak, J.A. Comments on the Seal Strength Requirements in the MSHA’s ETS on “Sealing of Abandoned Areas”, submitted to the Mine Safety and Health Administration, 2007.
24. Zipf, R.K., Sapko, M. J., and Brunde, J.F. *Explosion Pressure Design Criteria for New Seals in U.S. Coal Mines*. NIOSH Information Circular 9500, July 2007, 76 p.
25. Ju, Y., Law, C.K. Propagation and Quenching of Detonation Waves in Particle Laden Mixtures. *Combustion and Flame*, 129, 2002, 356-364.
26. Carvel, R.O., Thomas, G.O., Brown, C.J. Some observations of detonation propagation through a gas containing dust particles in suspension. *Shock Waves*, 13, 2003, 83-89.
27. Zhang, F., Gronig, H., van de Ven, A. DDT and detonation waves in dust-air mixtures. *Shock Waves*, 11, 2001, 53-71.
28. Papalexandris, M. Influence of inert particles on the propagation of multidimensional detonation waves. *Combustion and Flame*, 141, 2005, 216-228.
29. Barczak, T. Personal Communication, 2008.
30. The Mine Safety and Health Administration. Report of Investigation on Fatal Underground Coal Mine Explosion, January 2, 2006, Sago Mine, Wolf Run Mining Company, 2007, 190 p.
31. National Institute of Standards and Technology. Mechanical Properties of Structural Steels, NIST NCSTAR 1-3D, 2005, 288 p.